IMPROVING THE CAPACITY OF COSMO-SAC IN PREDICTING THE ACTIVITY COEFFICIENT OF IONIC LIQUIDS AT INFINITE DILUTION

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DECLARATION

I declare that the work in this dissertation titled 'Improving the Capacity of COSMO-SAC in Predicting the Activity Coefficient of Ionic Liquids at Infinite Dilution' has been conducted by me in the Department of Chemical Engineering. The information derived from literature has been duly acknowledged in the text and a list of references provided.

_____ _____

Danny James Akpan Date

CERTIFICATION

This dissertation entitled 'Improving the Capacity of COSMO-SAC in Predicting the Activity Coefficient of Ionic Liquids at Infinite Dilution' by Danny James Akpan meets the regulations governing the award of the degree of Master of Science of the Ahmadu Bello University and is approved for its contribution to knowledge and literary presentation.

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ABSTRACT

A new approach for improving the accuracy of infinite dilution activity coefficient (IDAC) of organic solutes in ionic liquids using COSMO-SAC was investigated in this research. The accuracy of Infinite Dilution Activity Coefficient of solutes in ionic liquids determined by the original COSMO-SAC model has been improved by modifying the model and fitting the adjustable parameters with experimental data from the National Institute of Standards and Technology (NIST). To carry out the fitting, sigma profile of ionic liquid cations and anions were first created using Dmol3 module in 2017 Accelrys Materials Studio and Sigma Averaging program. The sigma profile of the solutes was obtained from the VT-Database. The exchange energy expression was modified by including segment interaction parameters C_1 and C_2 to account for the charges on cations and anions, as well as the non-electrostatic contribution Cne to ascertain its effect on the systems. The standard segment surface area, a_{eff}, standard surface area in Staverman–Guggenheim equation, q, standard volume in Staverman–Guggenheim equation, r, segment interaction parameters C_1 and C_2, and the non-electrostatic contribution, C_{ne}, were fitted to 414 experimental data points using least square curve fitting program in Matlab. The data points were composed of 38 solutes, 10 cations and 11 anions in a temperature range from 288.15 to 395. 95K. The optimal values for the parameters a_{eff}, q, and r in the modified model from this work are 7.649 $Å^2$, 236.61$Å^2$ and 3.111 $Å^3$, respectively. Values for the hydrogen bond interaction coefficient C_{HB} and hydrogen bonding interaction cutoff charge σ_{HB} still remain 85580 and 8.4×10^{-3} respectively, as in the original model. The parameters C_1, C_2 and C_{ne} introduced to the model have been determined to be 3.415×10^{-14}, 1.278 and 5.06×10^{-2}, respectively. The calculated results agree with the experimental data within the Average Relative Deviation (ARD) deviation of 20.71%. The model from this work performs best for solutes with low polarity. Among the solutes used in this work, the model performed best for Alkynes, with ARD of 5.91%, while the poorest result was recorded for Water with ARD of 98.75%.

The ARD of IDAC from 29 data points which were not included in the parameter optimization was computed using the modified model to be 18.07%. In terms of Henry's law constant calculation for CO_2 in ionic liquids, the ARD of COSMO-SAC model from this work is 24.2% for 17 data points, as against that from COSMO-SAC 2010 which is 21.5%. Henry's law constant for CO_2 in 1-butyl-3-methyl-imidazolium bis(trifluoromethylsulfonyl)-amide [BMIM][TF_2N] and in 1-ethyl-3-methyl-imidazolium bis(trifluoromethylsulfonyl)-amide [EMIM][TF_2N] was also in good agreement with the experimental values at temperatures below the critical temperature of CO_2. The IDAC of benzene in ionic liquid of the type 1-alkyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide at 313.15K varied with chain length of the alkyl group as follows: $IDAC_{methyl} > IDAC_{ethyl} > IDAC_{butyl} > IDAC_{hexyl}$ while the IDAC of benzene in 1-ethyl-3-methylimidazolium-anion at 323.15K and 333.15K varied with anion size as follows: IDAC of Benzene: $IDAC_{TF2N} > IDAC_{EtSO4} > IDAC_{MeSO3}$.

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LIST OF SYMBOLS

γ	Activity coefficient
f	Pure component fugacity
$\hat{f}$	Fugacity of component in solution
∞	Infinite dilution
γ_i^{∞}	Activity coefficient at infinite dilution
β_{ij}^{∞}	Selectivity at infinite dilution
i, j, k, s	Chemical species
k_j^{∞}	Capacity at infinite dilution
H_i	Henry's law constant
P_i^*	Partial vapour pressure
T	Temperature
R	Gas constant
P	Pressure
n	number of moles
V_N	Net retention volume
v'^*_i	Liquid molar volume of the solute at its partial vapor pressure
v_i''	Partial molar volume at infinite dilution at the column pressure.
t_i	Retention time
K_i	Partition coefficient
x	Mole fraction
a, b	Phases
σ	Surface charge density

$A_i(\sigma)$	Surface area of specie with a charge density of value σ
A_i	Total surface area of specie
r_{eff}	Radius of the standard surface segment
r_n	Radius of the segment n
d_{mn}	Distance between segments m and n
E_{pair}	Self-energy of a segment pair
E_{mf}	Electrostatic interactions
E_{hb}	Hydrogen-bonding interactions
E_{ne}	Non-electrostatic interaction
C_{ne}	Non-electrostatic energy pair
α'	Misfit energy constant
ΔW	Exchange energy
ϵ_o	Permittivity of free space
a_{eff}	Standard segment surface area
C_{hb}	Hydrogen bonding interaction coefficient
σ_{HB}	Hydrogen bonding interaction cutoff charge
Q	Standard surface area in Staverman–Guggenheim equation
R	Standard volume in Staverman–Guggenheim equation
N	Number of data points
i	Chemical specie (used as subscript)

ABBREVIATIONS

ARD	Average Relative Deviation
ASOG	Analytical Solutions of Groups
BASIL	Biphasic Acid Scavenging utilizing Ionic Liquids
Bin	Binary
Calc	Calculated
CG	Carrier gas
COSMO-RS	Conductor-like Screening Model for Real Solvents
COSMO-SAC	Conductor-like Screening Model Solvation Activity Coefficient
DCT	Double Cell Technique
DISQUAC	Dispersive Quasi Chemical
Expt	Experimental
FILs	Fluorinated Ionic Liquids
GC	Gas Chromatography
GCM	Group Contribution Method
GLC	Gas-Liquid Chromatography
IDAC	Infinite dilution activity coefficient
IGST	Inert Gas Stripping Technique
IL	Ionic Liquid
LLE	Liquid-Liquid Equilibrium
LSER	Linear Solvation Energy Relationship
MOSCED	Modified Separation of Cohesive Energy Density
NIST	National Institute of Standards and Technology
NRTL	Non-Random Two-Liquid

OF	Objective Function
PI	Performance Index
RMSD	Root Mean Square Deviation
SCT	Single Cell Technique
SMs	Solvation Models
Tern	Ternary
UNIFAC	UNIQUAC Functional-group Activity Coefficients
UNIQUAC	Universal Quasi Chemical
VLE	Vapour-Liquid Equilibrium
WRMSD	Weighted Root Mean Square Deviation

CHAPTER ONE

1.0 INTRODUCTION

1.1 Background

Lei, *et al* (2017) described Ionic Liquids (ILs) as salts that have melting points below 100 ℃. They are wholly composed of cations and anions. Singh and Savoy (2020) and Welton (2018) in their works explained that salts that are liquids at room temperature are generally called room-temperature ionic liquids (RTILs). Ionic liquids have become a popular area of research in the past few years due to their very useful physical and chemical properties. It is therefore important to develop methods of determining their thermodynamic properties, of which activity coefficient is the focus of this work. Activity coefficients at infinite dilution provide a useful tool for solvent selection in extractive distillation or extraction processes, as discussed by Eckert and Sherman (1996).

Infinite Dilution Activity Coefficient (IDAC) for gaseous and liquid mixtures can be calculated using several methods, such as, UNIQUAC Functional-group Activity Coefficients (UNIFAC), Analytical Solutions of Groups (ASOG), Non-Random Two-Liquid (NRLT), Universal Quasi Chemical (UNIQUAC), or Conductor-like Screening Model Solvation Activity Solvents (COSMO-SAC), in the works by Gmehling, *et al* (1993), Tochigi *et al* (1990), Renon and Prausnitz (1968), Abrams and Prausnitz, (1975), and Lin and Sandler (2002), respectively. The COSMO-SAC approach has a major advantage over the other methods in terms of simplicity in that the calculations only require the knowledge of a structural formula and certain model parameters which is available in the relevant literature such as Xiong, *et al* (2014).

In this work, the COSMO-SAC model was reparametrized for IDAC predictions of solutes in ILs at different temperatures using experimental data from the National Institute of Standards and

Technology (NIST) database. The result from the reparametrized model was compared with the experimental data by calculating the Average Relative Deviation (ARD) of the modified model from the experimental data.

1.2 Problem Statement

One of the limitations to researching applications of the large possible combinations of ionic liquids is the cost of experiments. COSMO-SAC offer a very attractive starting point to screening the ionic liquids of interest before proceeding to laboratory experiments. However, COSMO-SAC does not always provide good prediction accuracy compared to the experimental results. Hence, there is a need to improve the accuracy of the COSMO-SAC method to predict Infinite Dilution Activity Coefficient (IDAC) of solutes in ionic liquids.

1.3 Aim and Objectives

The aim of this work is to improve the capacity of the COSMO-SAC model in predicting the IDAC of solutes in ILs.

The specific objectives are to:

i. Generate Sigma Profiles of solutes that are required in the work but not in the Virginia State University Database, VT-2005, as described in Mullins, *et al* (2006), as well as IL cations and anions.
ii. Modify and optimize the adjustable parameters of the COSMO-SAC model.
iii. Validate the improved model.
iv. Use the modified COSMO-SAC from this work to calculate Henry's law constants.
v. Study the effect of molecular structure of cation and anion on IDAC.

1.4 Justification

Ionic Liquids is currently attracting a lot of interest as an area of research due to the unique physical and chemical properties of this group of chemical compounds. A more accurate model for predicting IDAC of solutes in Ionic Liquids will no doubt be of tremendous use to chemical engineers in process simulation, plant design, process calculations, etc. Apart from screening of ionic liquids for tailored applications, the model can also be used to test the thermodynamic properties of hypothetical Ionic Liquid cations and anions from their chemical structures before they are synthesized.

1.5 Scope

This work is focused on improving the COSMO-SAC model for binary systems of the solute and Ionic Liquid. The ionic liquid shall be treated as wholly dissociated cations and anions. The COSMO-SAC 2002 programme which is available on Virginia Tech University website as a Fortran programme has been translated to Matlab programme for convenience (See Appendix D).

CHAPTER TWO

2.0 LITERATURE SURVEY

2.1 Background

The literature review covers previous works to understand their significance, and the contribution of the present study. The areas reviewed can be generally categorized into the following themes:

i. Ionic Liquids and their application in the chemical industry.
ii. IDAC and the importance of IDAC data.
iii. Measurement of Infinite Dilution Activity Coefficient (IDAC).
iv. The COSMO-SAC method.
v. Factors affecting IDAC (molecular structure, temperature).
vi. Accuracy of predictive models and improvements.

2.2 Ionic Liquids

Ionic Liquids have received much attention over the last two decades due to their unique properties such as low vapour pressure, tunability, solvation properties for organic and inorganic compounds, etc.

2.2.1 Properties of ionic liquids

A lot of research has been done into the properties and applications of Ionic Liquids. Some of these properties and applications have been reviewed in the article by shah *et al* (2020). They include:

i. Low vapour pressure.
ii. Relatively lower flammability hazard.
iii. Tunability.
iv. Good solvation properties.

v. High electric conductivities.

vi. High thermal stability.

vii. Wide liquid range.

viii. Wide electrochemical window.

According to Earle, *et al* (2006) Ionic liquids are generally known to be environmentally benign due to their low volatility, but some of them are volatile, and others are flammable, as seen in Smiglak, *et al* (2006).

2.2.2 Use of ionic liquids as solvents in separation processes

The large number of possible ion combinations makes it possible to design an ionic liquid with the desired properties to suit a particular application. One can adjust and tune ionic liquids by varying either the anion or cation, or both to provide a specific property, including density, melting point, viscosity, hydrophobicity, miscibility, and selectivity in separation processes. Table 2.1 highlights more advantages of ionic liquids over molecular solvents that have enhanced their popularity.

Table 2.1: Ionic liquids versus molecular solvents

Property	**Organic solvents**	**Ionic liquids**
Number of solvents	1000	1,000,000
Applicability	Single function	Multifunction
Catalytic ability	Rare	Common and tunable
Chirality	Rare	Common and tunable
Vapour pressure	Obeys Clausius-Clapeyron equation	Negligible vapour pressure under normal conditions
Flammability	Usually, flammable	Usually, non-flammable

Solvation	Weak solvating	Strongly solvating
Polarity	Conventional polarity concepts	Polarity concept questionable
Tunability	Limited range of solvent available	Virtually unlimited range means "Designer solvents"
Cost	Normally cheap	Typically, between 2 and 100 times the cost of organic solvents
Recyclability	Green imperative	Economic imperative
Viscosity (cP)	0.2 – 100	22 – 40,000
Density (g/cm^3)	0.6 – 1.7	0.8 – 3.3
Refractive index	1.3 – 1.6	1.5 – 2.2

Source: Plechkova and Seddon (2008)

2.2.3 Commercial applications of ionic liquids

Some of the commercial achievements publicly reported by Plechkova and Seddon (2008) regarding industrial uses of ionic liquids include:

i. Biphasic Acid Scavenging Utilizing Ionic Liquids (BASIL) Process
ii. Isobutene alkylation
iii. Dimersol Process
iv. Pharmaceutical intermediate production by Central glass Co, Ltd in Japan
v. 2, 5-dihydrofuran production by Eastman Chemical Company from 1996 to 2004
vi. Production of lithium-ion rechargeable battery by Pionics in Japan.

2.2.4 Potential applications of ionic liquids in the chemical industry

The properties of a given ionic liquid are determined by the nature of its ions. Hence, any desired set of properties can be imparted to an ionic liquid by a proper selection of the anion-cation pair.

This tunability of ionic liquids properties allows a very wide range of applications as shown in the table 2.2.

Table 2.2: Potential applications of ionic liquids in the chemical industry (Source: Plechkova and Seddon, 2008)

Chemical engineering	**Electrochemistry**	**Biochemistry**
Mass separation agents	Electrolyte batteries	Biomass processing
Catalyst	Metal plating	Drug delivery
Coatings	Solar panels	Personal care
Lubricants	Fuel cells	Biocides
Plasticizers	Electro-optics	Embalming
Dispersing agents		

2.3 Infinite Dilution Activity Coefficient (IDAC or γ^{∞})

According to IUPAC (1997), activity coefficient of a chemical specie $(\gamma_{i,}$ where i refers to the chemical specie$)$ is a measure of non-idealities in a liquid system composed of two or more chemical species. It is defined by equation 2.1.

$$\gamma_i = \frac{\hat{f}_i}{x_i f_i} \tag{2.1}$$

Where $\hat{f}_i$ is the fugacity of component *i* in solution, f_i its pure component fugacity, and x_i its molar fraction.

Infinite Dilution Activity Coefficient (IDAC),

γ_i^{∞}, also known as Limiting Activity Coefficient is the limiting value of the activity coefficient of a solute when its concentration tends towards zero, as expressed in equation 2.2.

$$lim(\gamma_i)_{x\to 0} = \gamma_i^{\infty} \quad (2.2)$$

2.4 Importance and Use of IDAC Data

According to Raal and Mühlbauer (1998). The infinite dilution region of solutions attracted much interest for some reasons underlining its great importance:

i. The system behavior in the very dilute regions is instrumental in obtaining high purity products.
ii. The most difficult and costly stage of a separation process is the removal of the last traces of impurity.
iii. The greatest departure from ideality occurs in the very dilute regions.
iv. Environmental concerns are based on the much-diluted regions in the gas phase which is air.

IDAC data is used for so many calculations like selectivity, distribution constant, capacity, etc., which are very useful in process design. A wide variety of separation processes such as distillation, Liquid-Liquid Extraction, chromatography, pharmaceuticals, wastewater purification, etc. require γ∞ values in their design.

2.4.1 Selectivity and capacity

The selectivity of a separating agent (or solvent) is its ability to preferentially separate a particular chemical specie that is in mixture with two or more species. The potentially best separating agent, called entrainer, is the one allowing the highest selectivity and capacity values. In other words, when solvents are investigated to find out the most suitable separating agent for a mixture containing two components *I* and *j*, their respective IDAC values in each solvent are determined. Equation (2.3) is then used to calculate the selectivity at infinite dilution β_{ij}^{∞} of each solvent with respect to the *i/j* system.

$$\beta_{ij}^{\infty} = \frac{\gamma_{is}^{\infty}}{\gamma_{js}^{\infty}} \tag{2.3}$$

γ_{is}^{∞} and γ_{js}^{∞} represent the limiting activity coefficients of *i* and *j* respectively in the solvent, *s*. β_{ij}^{∞} is the limiting selectivity of solvent *s* for the system consisting of components *i* and *j*. Thus, selectivity values at infinite dilution are important for a preliminary selection of an entrainer.

A second quantity to look at is the solvent capacity at infinite dilution, k_j^{∞}, which is numerically the maximum amount of species j that can be dissolved in the solvent, as shown in equation 2.4.

$$k_j^{\infty} = \frac{1}{\gamma_j^{\infty}} \tag{2.4}$$

Additionally, capacity reveals how much solvent is used during the separation process. The greater the solvent capacity, the smaller the amount of solvent used. In principle, the solvent to use as separating agent is supposed to have the highest value of both selectivity and capacity. But in practice, a compromise is to be found, since these two quantities are in inverse variation with respect to one another. According to Kumar and Banerjee (2009), a criterion that incorporates both selectivity and capacity together is called performance index, given by the product of these properties. Thus, at infinite dilution, Performance Index (PI^{∞}) is expressed by equation 2.5.

$$PI^{\infty} = \beta_{ij}^{\infty} k_j^{\infty} \tag{2.5}$$

The determination of γ_i^{∞} permits one to evaluate the potential use of solvents. Therefore, it serves as a pre-selection criterion.

2.4.2 Henry's law constants

The relationship between the Henry's law constant of a solute in a solvent and its limiting activity coefficient is expressed in equation 2.6.

$$\gamma_i^{\infty} = \frac{H_i}{P_i^*} \tag{2.6}$$

H_i represents the Henry's law constant for solute *i* in the solvent and P_i^* is the vapour pressure of solute *i* at the temperature for which the IDAC is determined. Equation (2.6) shows that Henry's law constants can be found through IDAC values. According to Eike *et al* (2004), in cases where the temperature of the system is above the critical temperature of the solute the Henry's law constant, rather than the IDAC is useful Design calculations for gas separation applications commonly involve the use of Henry's law constants.

2.5 Measurement of IDAC

In this section, the different methods of measuring IDAC will be reviewed and some of their strengths and weaknesses will be discussed.

2.5.1 Experimental methods

The experimental methods include Gas Chromatography, Differential Static Cell, Differential Ebulliometry, Dew Point Method, Partition Coefficient, and Inverse Solubility,

I. Gas Chromatography

In the Gas Chromatography method proposed by Sandler, *et al* (1996), the solvent is loaded onto a chromatograph column and a small amount of solute for which it was intended to measure it's γ^{∞} is injected into the carrier gas. Considering the simplest case of low total pressure so that all gas-phase non-idealities can be neglected, equation 2.7 gives the relationship between the natural logarithm of activity coefficient at infinite dilution and temperature, number of moles, retention time, liquid molar volume, and vapour pressure.

$$ln\gamma^{\infty}(T) = ln\left[\frac{n_3^1 RT}{V_N P_1^*}\right] + \frac{v_1^* P_1^*}{RT} - \frac{v_1'' P}{RT} \qquad (2.7)$$

Where n_3 is the number of moles of solute on the column, V_N, is the net retention volume of the solute-loaded column, v'^*_1 is the liquid molar volume of the solute at its vapor pressure P^*_1, and v''_1 its partial molar volume at infinite dilution at the column pressure P.

The main difficulties with this method are in determining the number of moles of solvent on the column at any time, and the net retention volume, that is the volume of gas passing through the column between the injection and elution of the solute (Sandler, *et al* (1996)).

In a simpler method, if two (or more) solutes are injected onto a solvent-loaded GC column simultaneously, and it is recognized that each net retention volume is proportional to the net residence time in the column (the actual residence time less that of an inert gas), then it can be shown that:

$$\frac{\gamma_1^\infty}{\gamma_2^\infty} = \frac{P_2^*}{P_1^*}\alpha_{21} = \frac{P_2^*}{P_1^*}\frac{t_2 - t_{in}}{t_1 - t_{in}} \tag{2.8}$$

Where t_1 is the retention time of species i and t_{in} is the retention time from a non-absorbing gas. Consequently, if one has obtained the easily measured retention times t_{in}, t_1 and t_2, and knows the vapor pressures of both components, and the infinite dilution activity coefficient of one of the components in the solvent, the infinite dilution activity coefficient of the other component is easily obtained. Also, since the Henry's law coefficient (on a mole fraction basis) is shown in equation 2.9.

$$H_i(T) = \gamma_i^\infty P_i^*(T) \tag{2.9}$$

Even if the vapor pressure of the second component is not known, its Henry's law coefficient can be obtained from equation 2.10.

$$H_i(T) = \gamma_2^\infty P_2^*(T)\alpha_{21} = H_2(T)\alpha_{21} \tag{2.10}$$

Some advantages of Gas Chromatography include:

i. The measurements are rapid.
ii. They require simple equipment.
iii. They require only small amounts of chemicals, and
iv. The purity of the solute is not crucial.

However, there are several limitations to this method which include:

i. The solute must be more volatile than the solvent, and the method works best if it is much more volatile.
ii. There are frequently adsorption problems at surfaces and interfaces, especially with polar and protic compounds.
iii. Some chromatographic detectors are inapplicable to some solutes.

II. Differential Static Cell Method

In this method of determining γ^{∞}(Sandler, *et al* (1996)), the pressure difference is measured quite accurately between a pure solvent and a very dilute solution, mutually thermostatted. The change in equilibrium pressure *dP* due to the very small (generally gravimetric) addition of a second component resulting in a differential composition change dx is measured. The value of γ^{∞} is then computed at low pressure using equation 2.11.

$$\gamma_2(x_2 \to 0) = \gamma_2^{\infty} = \frac{P_1^* + \left(\frac{\partial P}{\partial x_2}\right)_{T, x_1 \to 0}}{P_2^*} \tag{2.11}$$

This method has the advantage of being very accurate in that it is a difference method. However, the limitations include:

i. The solute must be fully degassed.

ii. The vapor pressure of the solute must be sufficiently high to make a measurable contribution to the total pressure of the mixture, and

iii. The partial volatilization into the vapor space that results in the liquid composition of the static cell being different than the gravimetrically prepared value, especially for highly volatile solutes must be accounted for.

III. Differential Ebulliometry

In this method, the change in boiling temperature (dT) with small changes in composition (dx) is measured (Sandler, *et al* (1996)). The vapor spaces over both boiling liquids are in contact with each other and thus at the exact same pressure. The measured slope of the change in boiling temperature with respect to composition is used to determine the γ^{∞}. The expression for this is shown in equation 2.12.

$$\gamma_2(x_2 \to 0) = \gamma_2^{\infty} = \frac{P_1^* - \left(\frac{dP_1^*}{dT}\right)\left(\frac{\partial T}{\partial x_2}\right)_{P,x_2 \to 0}}{P_2^*} \tag{2.12}$$

Unlike Gas Chromatography, this technique can be used to determine γ^{∞} in systems where both components have similar volatilities, and even works best when the relative volatilities are not very different, although this can be a limitation if the measurement is to be made for species with volatilities that are wide apart. This technique can be run over wide ranges of pressure and temperatures, and like the Differential Static Cell Method, the ebulliometry is a difference method.

IV. Dew Point Method

This method complements the ebulliometric method well (Sandler, *et al* (1996)). A solvent, or solution of known composition is vaporized and thermostatted, then allowed to impinge on a thermostatically controlled optical dew point sensor. This device employs a thermoelectric cooler to cool a small metal mirror until a thin film of condensation on the mirror is detected by laser light scattering. This experiment is excellent for systems with very low relative volatilities, which

are mathematically difficult for the ebulliometer technique and are not measurable by gas chromatography. One major limitation of this method is that it has not been successfully applied to aqueous systems outside the temperature range of 10-75°C.

V. Partition Coefficient and Inverse Solubility

Partition coefficient of liquids and liquid-liquid solubility measurements can also be used to find γ^{∞} values (Sandler, *et al* (1996)).

If there are two liquid phases, and a very small amount of solute is added to the two-phase mixture and then the compositions of the solute in both phases are measured, from the equality of fugacities, it is easily shown from equation 2.13 that the ratios of the mole fraction or activity coefficient of the solute in the two phases I and II or II and I, respectively, is equal to the partition coefficient.

$$K_i = \frac{x_i^I}{x_i^{II}} = \frac{\gamma_i^{II}}{\gamma_i^I} \tag{2.13}$$

where *K*, is the partition coefficient, x_i^I and x_i^{II} are the mole fractions of solute i in phase I and II respectively, γ_i^I and γ_i^{II} are the activity coefficients of solute i in phase I and II, respectively. If the solute concentrations are sufficiently diluted, then *K* is the ratio of the infinite dilution activity coefficients that is obtained. Therefore, if the infinite dilution activity coefficient of a specie in one of the phases is known, the value of its infinite dilution activity coefficient in the other phase can be obtained from the partition coefficient, provided the two liquids are immiscible in each other e.g., benzene and water.

For Inverse Solubility method, the start is to express the two phases of liquids that are in equilibrium by:

$$x_2^a \gamma_2^a = x_2^b \gamma_2^b \tag{2.14}$$

where a and b phases are each almost pure component 1 and 2, respectively. Thus, to a very good approximation, $x_2^b = 1$ and $\gamma_2^b = 1$, and γ_2^∞ is the inverse of the solubility in the 1-rich phase.

$$\gamma_2^\infty = \frac{1}{x_2^a} \tag{2.15}$$

According to Eckert and Sherman (1996), for equation 2.15 to be used, the solubility should be low. However, the accurate measurement of solubility for compounds with low solubility can be challenging (Sandler, *et al* (1996)).

2.5.2 Predictive methods

The predictive methods are mainly divided into two: the Group Contribution Methods and Ab Initio Methods (Which mainly comprise of the COSMO-based methods)

1. *Group Contribution models*

UNIFAC (Gmehling and Schiller, (1993)) and ASOG (Tochigi, *et al* (1990)) are the most popular group contribution methods for liquid phase activity coefficients. The idea behind group contribution methods is that organic molecules which belong to a given homologous series contain varying numbers of the same kind of segments or groups. It is assumed that the interaction energy between molecules really depends upon the interactions between individual groups that compose the molecules. With this assumption, the configurational energy between molecules is given by the sum of all the group interaction energies. By using the group-contribution method the properties of a great number of systems can be calculated with only a relatively small number of group interaction parameters.

The major shortcomings of all of group contribution methods include:

i. They do not work well for aqueous systems. Due to its unique structure and hydrogen-bonding characteristics, water often exhibits quite non-ideal behavior as compared to the behavior of other solvents.

ii. They require experimentally determined parameters.

iii. They are unable to differentiate the different isomers of molecules.

2. COSMO-base Methods

The conductor–like screening model (COSMO) is a predictive method for thermophysical properties using a quantum chemical approach. The two most widely used COSMO-based variants for infinite dilution activity coefficients in ionic liquids are COSMO-RS (The conductor–like screening model for real solvents), developed by Klamt and Eckert (2000) and COSMO-SAC (The conductor–like screening model, solvation activity coefficients) developed by Lin and Sandler (2002). These two models involve statistical thermodynamics, along with quantum chemical calculation. They require σ-profiles of molecules in the same manner as group contribution methods rely on group interaction parameters (Dohnal, *et al* (2008)). Some of the advantages of COSMO-based methods over semi-empirical methods like UNIFAC and UNIQUAC are:

i. Ability to differentiate isomers: A special ability of the COSMO-based methods to differentiate isomers makes it more desirable for such applications. This is because the σ-profile is unique to each chemical structure.

ii. The use of fewer adjustable parameters: Unlike group contribution methods, COSMO-based methods do not require a unique set of experimentally determined parameters for each molecule. Once the model parameters are optimized using experimental data for certain groups of compounds, the only starting input required for property prediction is the

chemical structures of the molecules. Where reliable sigma profiles are available, they can be used directly for the calculations instead of generating them from the chemical structure.

2.6 COSMO-SAC Theory

In the COSMO-SAC model (Lin and Sandler (2002)), the surface of each molecule is divided into segments and the screening charge density corresponding to each segment is calculated. This three-dimensional charge distribution is projected to a two-dimensional histogram by calculating the probability of finding a segment having a screening charge density σ. This probability distribution $p_i(\sigma)$ is known as the sigma profile.

$$p_i(\sigma) = \frac{A_i(\sigma)}{A} \tag{2.16}$$

where:

$A_i(\sigma)$ is the surface area of specie with a charge density of value σ.

A_i is the total surface area of species i.

For a mixture, the σ-profile is determined from the area-weighted average of contributions from all the components present in the mixture. This is given as

$$p_s(\sigma) = \frac{\sum_i x_i A_i p_i(\sigma)}{\sum_i x_i A_i} \tag{2.17}$$

where x_i is the mole fraction of component i in the mixture.

Since different surfaces have different number of segments, the following algorithm is used to obtain apparent screening charges to be used in the original COSMO-SAC model:

$$\sigma_m = \frac{\sum_n \sigma_n^* \frac{r_n^2 r_{eff}^2}{r_n^2 + r_{eff}^2} exp\left(-\frac{d_{mn}^2}{r_n^2 + r_{eff}^2}\right)}{\sum_n \frac{r_n^2 r_{eff}^2}{r_n^2 + r_{eff}^2} exp\left(-\frac{d_{mn}^2}{r_n^2 + r_{eff}^2}\right)} \quad (2.18)$$

Where:

$r_{eff} = \sqrt{a_{eff}/\pi}$ is the radius of the standard surface segment

$r_n = \sqrt{a_n/\pi}$ is the radius of the segment n

d_{mn} is the distance between segments m and n

The sigma profiles of the various components are used in a thermodynamic model to calculate the activity coefficients of the components in each solution.

The self-energy of a segment pair E_{pair} necessary for the calculation of the solvation activity coefficients contains contributions from the electrostatic interactions E_{mf}, the hydrogen-bonding interactions E_{hb} and non-electrostatic interaction, E_{ne}.

$$E_{pair}(\sigma_{m,}\sigma_n) = E_{mf}(\sigma_{m,}\sigma_n) + E_{hb}(\sigma_{m,}\sigma_n) + E_{ne}(\sigma_{m,}\sigma_n) \quad (2.19)$$

The non-electrostatic energy is assumed to be a constant C_{ne} term.

$$E_{pair}(\sigma_{m,}\sigma_n) = \frac{\alpha'}{2}(\sigma_m + \sigma_m)^2 + C_{hb}\max[0, \sigma_{ac} - \sigma_{hb}]\min[0, \sigma_{don} - \sigma_{hb}] + C_{ne} \quad (2.20)$$

Since it was assumed that the non-electrostatic energy pair cancel out, $C_{ne}\ becomes\ zero$, and the exchange energy becomes

$$\Delta W(\sigma_m, \sigma_m) = \frac{\alpha'}{2}(\sigma_m + \sigma_m)^2 + C_{hb}\max[0, \sigma_{ac} - \sigma_{hb}]\min[0, \sigma_{do} - \sigma_{hb}] \quad (2.21)$$

where α' is a constant for the misfit energy that is calculated from the surface area of a standard segment as follows.

$$\alpha' = \frac{0.64 \times 0.3 \times a_{eff}^{1.5}}{\epsilon_o} \tag{2.22}$$

$\epsilon_o = 2.395 \times 10^{-4}$ (Permittivity of free space)

Table 2.1: Values of parameters in COSMO-SAC method.

Parameters	Meaning	Values
a_{eff}	standard segment surface area	7.50 $Å^2$
C_{hb}	hydrogen bonding interaction coefficient	8.558×10^4 kcalmol^{-1} $Å^4$ e-^{2}
$\boldsymbol{\sigma_{HB}}$	hydrogen bonding interaction cutoff charge	0.0084 e$Å^{-2}$
Q	standard surface area in Staverman–Guggenheim equation	79.53 $Å^2$
R	standard volume in Staverman–Guggenheim equation	66.69$Å^3$

Source: Xiong, *et al* (2014).

2.7 Effect of Molecular Structure on Activity Coefficient

Several research works have established that relationships exist between the molecular structure of solutes, IL cations and anions, and the activity coefficient of the solutes at infinite dilution. P. Reddy, *et al* (2011) reported that the γ_{solute}^{∞} values are much higher for the hydrocarbon solutes than those associated with ILs with long alkyl chains and shorter alkyloxy groups, which indicates weaker hydrophobic interactions between the IL and the hydrocarbon solutes. The hierarchy for the γ_{solute}^{∞} values in decreasing order for the organic solutes are as follows:

n-alkanes > 1-alkenes > cycloalkanes > 1-alkynes > ketones > aromatic compounds > alcohols.

The availability of localized or delocalized pi electron clouds, lone pair electrons, and permanent dipoles enhance the affinity of the ionic liquid for organic solutes. Ionic liquids generally have

stronger interactions with water and the alcohol than for other classes (including ketones) due to favourable hydrogen-bonding interactions between the ILs cation and the hydroxyl group of the alcohols and water. For aromatic compounds, γ_{solute}^{∞} increases when carbon number of the alkyl component of the side chain on the benzene ring increases.

2.8 Temperature and Pressure Effects

Pressure generally has an insignificant effect on γ_{solute}^{∞} measurements. Recalling equation 2.1, we see in equation 2.23 that pressure equal to zero is also a part of the standard state (i.e., pure liquid solute at zero pressure). That is a hypothetical state of the solute.

$$lim(\gamma_i)_{x\to 0} = \gamma_i^{\infty}(P \to 0) \qquad 2.23$$

Krolikowski, *et al* (2021) reported that for measurements carried out in the temperature range from 318.15 to 358.15K, the natural logarithm of γ_{solute}^{∞} is a linear function of inverse temperature by the linear Van't Hoff relation. Equation 2.24 from Krolikowski, *et al* (2021) shows this expression.

$$\ln(\gamma_i^{\infty}) = \frac{a}{T} + b \qquad 2.24$$

The values for the constants a and b in equation 2.24 can be found in Krolikowski, *et al* (2021).

2.9 Effects of Chemical Structure on IDAC

The greater the electronegativity difference between atoms in a bond, the more polar the bond (http://chemistry.elmhurst.edu/vchembook/213organicfcgp.html. Accessed on 21 November 2021). Partial negative charges are found on the most electronegative atoms, the others are partially positive. In general, the presence of oxygen imparts more polarity than nitrogen because oxygen is more electronegative than nitrogen. Hydrocarbons are generally non-polar (or apolar) due to the combination of hydrogen, oxygen, and functional groups. A general polarity ranking for organic compounds can be summarized as follows:

Amide > Acid > Alcohol > Amine > Ether > Alkane

Carvalho, *et al* (2014) established that the smaller nitrogen atom has a higher electron density and therefore, is more strongly polarized than the larger phosphonium atom in IL cations. This causes a stronger cation-anion interaction and a more rigid liquid structure than the phosphonium equivalent, which makes the anion less mobile. The higher mobility of the anions in phosphonium ILs induces more intermolecular interactions with solutes and consequently a larger for the γ_{solute}^{∞} for non-polar solutes and slightly lower for polar solutes. This effect will be more significant at low IL molar weights, otherwise the intermolecular interactions of the ILs will be dominated by the alkyl tails.

2.10 Accuracy of Predictive Models

Several authors have published mixed results for accuracy of predictive models in IDAC prediction of ionic liquid systems. In this section, the relevant literatures shall be reviewed.

Brouwer, *et al* (2021) carried out a comprehensive work on the model performances for IDAC using UNIFAC, modified-UNIFAC (Do & Ly), COSMO-RS, MOSCED, Hildebrand model, and Abraham model. The accuracy of the predictive models was differentiated based on aliphatic, aromatic, halogen, aprotic polar, and protic polar compounds in the following solvents:

i. Molecular solvents: Aliphatic, Aromatic, Halogen, Aprotic polar and Protic polar compounds.
ii. Ionic liquids with various non-functionalized cations (Imidazolium, Pyrrolidinium, Phosphonium, Sulphonium) and Functionalized Cations (Imidazolium, Pyrrolidinium, Pyridinium, Morpholinium).
iii. Ionic liquids with various Anions.

A general selection criterion was proposed by Brouwer, *et al* (2021), as seen in Table 2.4.

Table 2.4: Overview of the most accurate predictive model of each specific category of binary molecular solvent – solute mixture.

	Solute				
Solvent	Aliphatic	Aromatic	Halogen	Aprotic Polar	Protic Polar
Aliphatic	Modified UNIFAC(Do)	Modified UNIFAC(Do)	`	COSMO-RS	Abraham
Aromatic	COSMO-RS	COSMO-RS	MOSCED	Abraham	UNIFAC
Halogen	MOSCED	MOSCED	COSMO-RS	MOSCED	Abraham
Aprotic polar	MOSCED	MOSCED	MOSCED	MOSCED	Abraham
protic polar	Abraham	MOSCED	Abraham	MOSCED	Modified UNIFAC(Ly)

Source: Brouwer, *et al* (2021)

Overall, the model choice for the most accurate γ^{∞}_{solute} should be determined based on the following considerations:

i. Table 2.4 may be used as a guide to choose a method if all molecular parameters of the chosen molecules are available in the literature.

ii. GCMs or COSMO-RS should be used for the prediction when the molecular parameters are lacking or are questionable (strongly deviating from the same parameters for comparable molecules).

iii. The Abrahams model is the most accurate model for ILs when the molecular parameters are known.

iv. The applicability of the method for the intended research should be taken into consideration. For example, GCMs and COSMO-RS can predict a much wider range of molecular properties than the SMs and LSER.

2.11 Parameter Optimization

Han, *et al*, (2018) was able to improve the accuracy of the COSMO-RS model for predicting the IDAC of solutes in ionic liquids by optimizing the adjustable parameters of COSMO-RS. They obtained significant improvements compared to the former models. The objective function was the Absolute Relative Deviation, and it was minimized to obtain new values for the model parameters. The objective function is expressed in equation 2.25.

$$OF = min\left\{\frac{1}{N}\sum_i^N \left|\frac{\gamma_i^{\infty,exp} - \gamma_i^{\infty,calc}}{\gamma_i^{\infty,exp}}\right|\right\} \tag{2.25}$$

where $\gamma_i^{\infty,exp}$ and $\gamma_i^{\infty,calc}$ are the experimental and calculated activity coefficients of solute *i* in ILs at infinite dilution. *N* is the number of data points.

Bharti *et al* (2017) reported that the COSMO-SAC model is more accurate in predicting the IL-free systems, indicating that this method still requires validation and further development.

It is important to note that IDAC calculations of ionic liquid systems using COSMO-SAC 2002 yields very large relative deviations from experimental results, which is probably why no such results have been published. Shah *et al* (2012) tried to correlate the experimental IDAC data by varying C_{hb} in the COSMO-SAC 2002 model. Their efforts were unsuccessful, until they used the 2007 model, which has a more fundamentally sound expression for the hydrogen bonding.

Bharti *et al* (2018) investigated the multicomponent LLE predictions by COSMO-RS of aromatic extraction systems. The overall RMSD is less than 5%, and the prediction is more accurate for systems without IL.

In recent studies, attempts have been made to develop a hybrid model which combines the ease of IDAC prediction offered by the COSMO-SAC model with the relatively high prediction accuracy of the UNIFAC model, called COSMO-UNIFAC model (Dong *et al*, 2020, Zhu *et al*, 2020, and

Dong *et al*, 2019). While this approach gives high accuracy IDAC calculations, the functional group parameters of new compounds (e.g., ionic liquid cations and anions), which are needed for IDAC prediction using UNIFAC need to be obtained from a regression of the parameters using IDAC obtained from COSMO-SAC.

CHAPTER THREE

3.0 MATERIALS AND METHODS

3.1 Materials

The following equipment and software were used in carrying out the research work:

i. Personal Computer (Windows 7 Professional 64bit Operating System, Intel Celeron – Dual Core@2.3GHz, 4GB RAM, 500GB HDD).
ii. Workstation Computer (Windows 10 Professional 64bit Operating System, Intel(R) Xeon(R), 8 Cores @1.70GHz, 32GB RAM, 1TB HDD).
iii. Matlab version 2020.
iv. Acceryls Materials Studio version 2017.
v. Chemical Structures of solutes and ionic liquid (cations and anions) from Chemspider, Pubchem and NIST webbook.
vi. IDAC Data (Temperature, Composition, Pressure, IDAC) from NIST webbook.
vii. Activity Coefficient and Sigma Averaging FORTRAN programme for COSMO-SAC 2002 (See Appendix D)

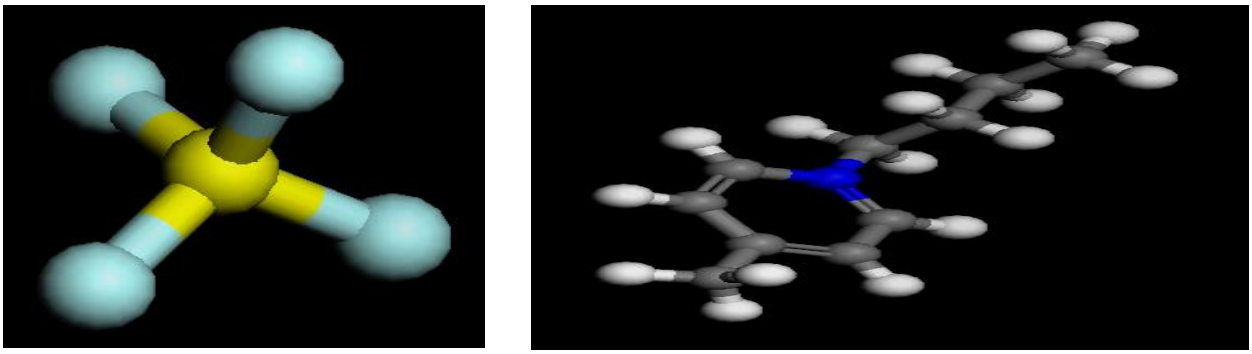
3.2 Methodology

3.2.1 Collection and preparation of IDAC experimental data

First, experimental IDAC values of solute in IL systems as well as the temperature of the system were collected from NIST website and stored in a Matlab file. The Matlab programme can easily call sigma profile files of the solute, cation, and anion, as well as read the system temperature and experimental IDAC value of solutes, all of which have been saved in the same Matlab folder.

3.2.2 Collection of Chemical Structures

The chemical structures of all the solutes, cations and anions collected in 3.2.1 were downloaded in '.mol' file format from chemspider, NIST webbook and pubchem websites. These structures will serve as the input structures in DMol for Geometry Optimization with visual display in Materials Studio is as seen in plate 3.1.



(a) (b)

Plate 3.1: Input structures for Geometry Optimization (a) tetrafluoroborate (b) 1-butyl-4-methylpyridinium (BMPY)

3.2.3 Geometry Optimization

To carry out the quantum chemical calculations, Dmol3 module in 2017 Accelrys Materials Studio was used to carry out the geometry optimization of the molecules to obtain their lowest energy configuration using density functional theory. The first step in this quantum chemical calculation involves creation of projects each for the solutes, cations and anions using the "3D atomistic model". This is followed by importing the ".mol" files previously downloaded in section 3.2.2 into each created project accordingly. Each molecule's structure is added with hydrogen if need be and cleaned.

To carry out the optimization, the GGA/VWN-BP functional (GGA represents the generalized gradient approximation, and VWN-BP represents the Becke–Perdew version of the Volsko–Wilk–

Nusair functional) setting and the DNP basis set v4.0.0 as recommended by previous works was used (Mullins *et al*, 2006).

The "Spin Unrestricted" was checked when working with cations and anions. This is necessary when working with radicals, charged molecules (IL cation and anion in this case), and organometallics as explained in the procedure for COSMO-SAC released by Lin *et al* in (2002). Also, the charge is set to 0, +1 or -1 for solutes IL cations and anions, as seen in plate 3.1. Note that these charges correspond to the charge number of the chemical species respectively.

After the geometry optimization, the output file containing the optimized geometry serves as the input for the energy calculation. An energy calculation is carried out using the same parameters as the geometry optimization, except that the extra cosmo radii parameters were added (see Appendix A for sample input files). At the end of the energy calculations, the cosmo files of the molecules was generated.

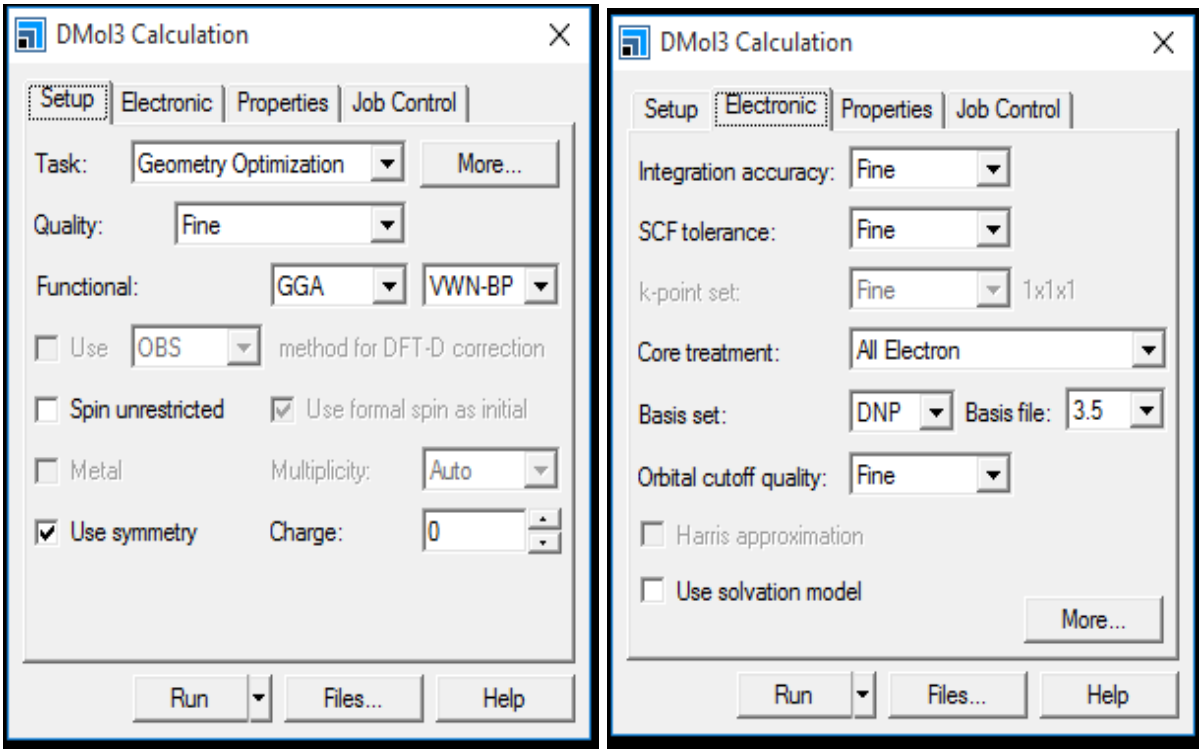


Plate 3.2: GUI for Geometry Optimization and Energy Calculations in DMol3 version 2017.

3.2.4 Sigma Profile Generation

The charges in the cosmo file generated in section 3.2.3 are averaged using the averaging programme provided by S.I Sandler and co. Note that the units of acosmo, vcosmo, and segment areas generated by Materials Studio version 2017 are in atomic unit (au) and must be converted to Angstrom (Å) by multiplying by 0.5292, to obtain accurate sigma profile calculation with this programme. The COSMO-SAC 2002 sigma averaging programme which was in FORTRAN was translated to Matlab for ease of programming (See Appendix D).

3.2.5 Activity Coefficient

Once the sigma profiles have been generated, the activity coefficients were calculated from the sigma profiles using the COSMO-SAC programme. The algorithm runs based on the equations in Section 2.6. The parameters to be optimized are prepared accordingly and the programme is run as a function file. The sigma profile, total surface area, total volume and component ID are useful information to calculate the activity coefficient of the molecule at a particular mole fraction and temperature. This programme was also translated to Matlab. (See Appendix D)

3.2.6 Parameter optimization

The adjustable parameters a_{eff} and C_{hb}, C_1, C_2 and C_{ne} were optimized to minimize the Average Relative Deviation (ARD) of the calculated IDAC values to the experimental values as outlined in equation 24, using LSQ Curve Fit Tool in Matlab. The original values of the parameters were used as the initial values for the optimization. The dataset for the optimization consisted of 414 data points of experimental IDAC values of solutes – IL systems from NIST (See Appendix B). The solutes and ionic liquids (cations and anions) used in the work are shown in table 3.1.

Table 3.1: Solutes, Cations and Anions used for the parameter optimization of the modified COSMO-SAC model.

	SOLUTES		**IL CATIONS**	**IL ANIONS**
Ethyl ethanoate	vinyl acetate	Dichloromethane	1-butyl-3-methyl-imidazolium	tetrafluoroborate
propane-2-ol	Pyridine	Thiophene	1-butyl-4-methyl-pyridinium	Chloride
Acetonitrile	tetrahydrofuran	Pentanal	1-butyl-1-methyl-pyrrolidinium	dimethylphosphate
Methanol	1-nitropropane	Butanal	1-ethyl-3-methyl-imidazolium	ethanesulfonate
propan-1-ol	acetone	Heptanal	Ethylpyridinium	ethyl sulfate
Ethanol	1,3-dimethylbenzene	methyl propanoate	1-hexyl-3-methyl-imidazolium	methanesulfonate (mesylate)
trichloromethane	1,4-dimethylbenzene	methyl pentanoate	1,3-dimethyl-imidazolium	methyl sulfate
tetrachloromethane	1,2-dimethylbenzene	methyl heptanoate	*n*,*n*,*n*,*n*-trimethylbutylammonium	hexafluorophosphate
pentan-2-one	ethylbenzene	Hexanal	1-octyl-3-methyl-imidazolium	tetracyanoborate
Butanone	toluene	Propanal	1-ethyl-2,3-dimethylimidazolium	bis(trifluoromethylsulfonyl)-amide
Water	benzene	methyl hexanoate	Pyridinium	Octylsulfate
1-hexyne	1-heptyne	methyl butanoate		methoxyethylsulfate
1,4-dioxane	Styrene			2-(2-methoxyethoxy) ethyl sulfate

3.2.7 Validation of data

The model was validated in three major ways: IDAC was computed using new data points not used in the parameter optimization, the effects of cation and anion size on IDAC, Henry's law constant computed using the modified model and COSMO-SAC 2010 (See Appendix C for data on validation). Figure 3.1 shows the process flow chart for this work.

I. IDAC calculation with new data points

After obtaining the new parameters from optimization, the COSMO-SAC model was reparametized with the new parameters and tested with a fresh set of 29 experimental IDAC data points from NIST which were not previously used for the optimization of the new parameters and the ARD was computed.

II. Effect of cation/anion size on IDAC

The effect of cation size on IDAC was studied by varying the chain length of the alkyl in benzene (1) - 1-Alkyl-3-MethylImidazolium bis[(trifluoromethyl)sulfonyl]imide (2) system at 313.15 K. Similarly, the anion was varied to test the effect of anion size in benzene (1) - 1-Ethyl-3-MethylImidazolium-Anion (2) system at 323.15K

III. Calculation of Henry's law constant

Henry's law constant of CO_2 in the ionic liquids was calculated using the improved model and benchmarked with a related work that used COSMO-SAC 2010 for the same calculations. Also, the effect of temperature on the accuracy of the model was studied. More details on the calculation can be found in Appendix C.

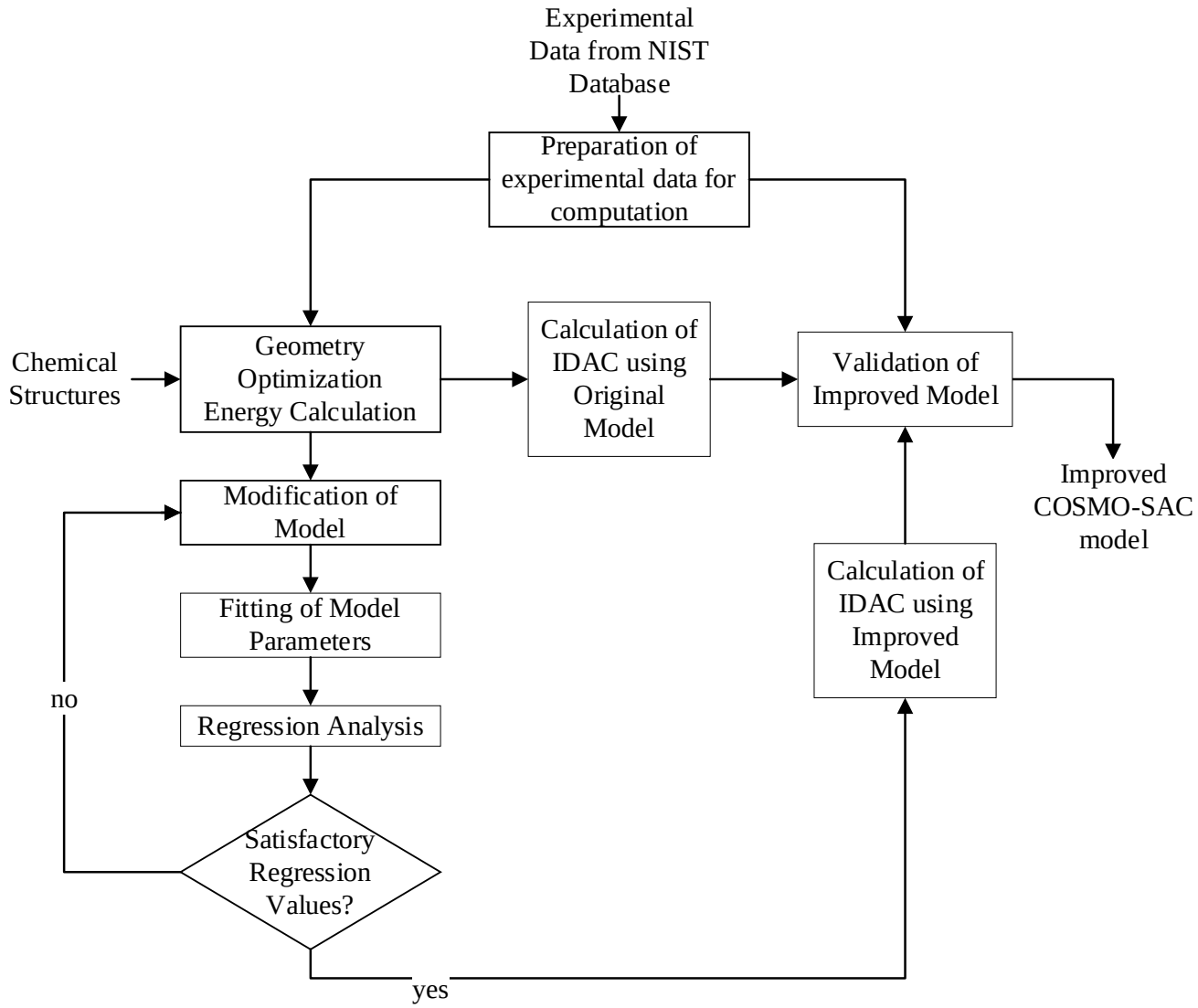


Figure 3.1: Process flow chart for the work

CHAPTER FOUR

4.0 RESULTS AND DISCUSSION

4.1 Sigma Profiles of Cations and Anions

In total, 38 solutes, 11 cations and 13 anions were used in this work, as seen in the previous chapter (Table 5). The sigma profile and solvation activity coefficients were divided into three areas by two vertical lines, σ = − 0.0082 e/Å2 and σ = + 0.0082 e/Å2. The middle part is the non-hydrogen bond region. The left side of σ = − 0.0082 e/Å2 is the H-bond donor region, and the right side of σ = + 0.0082 e/Å2 is the H-bond acceptor region. The σ-profiles for the IL cations and anions generated in this work are shown in figures 4.1 and 4.2, respectively.

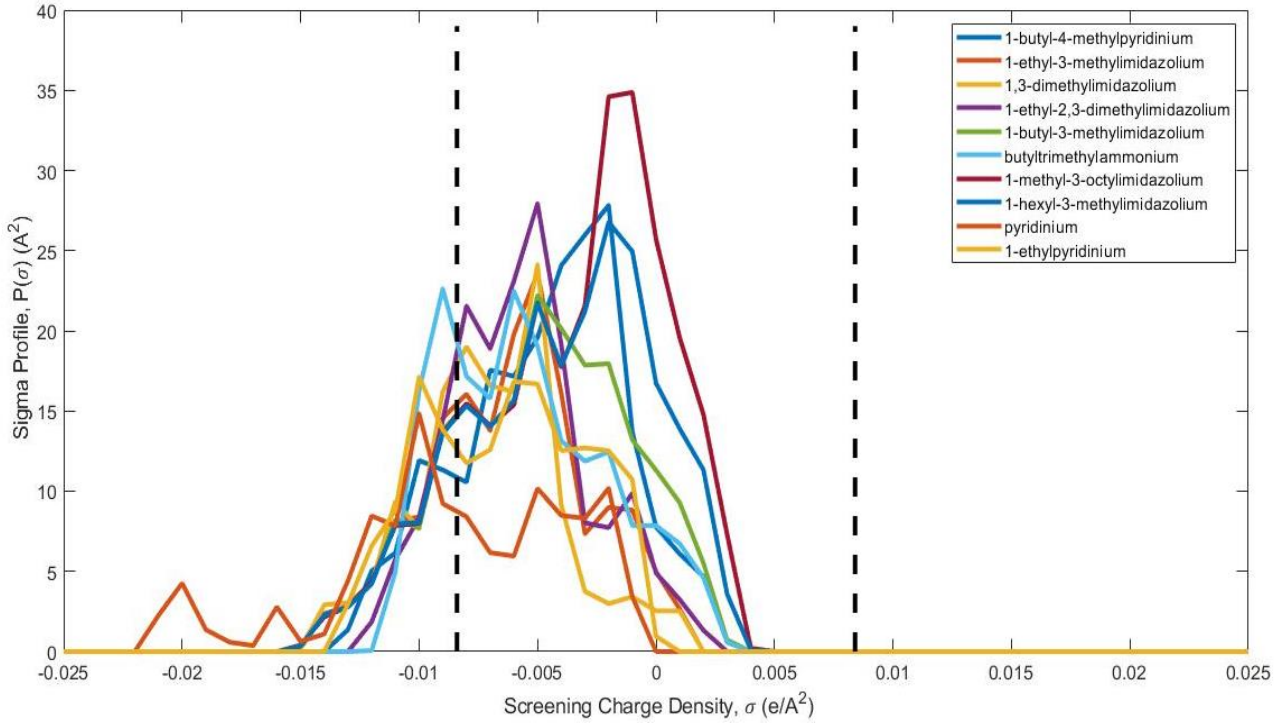


Figure 1: Sigma Profile of cations used in this work.

The shape and range for all the studied cations are similar. Their *σ*-profiles contains one main peak located in the non-hydrogen bond region, reaching the H-bond donor region (Figure 4.1). In like manner, the shape and range for all the studied anions are also similar. They contain one main peak in the non-hydrogen bond region, reaching the H-bond acceptor region (Figure 4.2). The similarity

in shape and range of cations and anions is an indication that the ions have similar polarity and the ability to form hydrogen bonds.

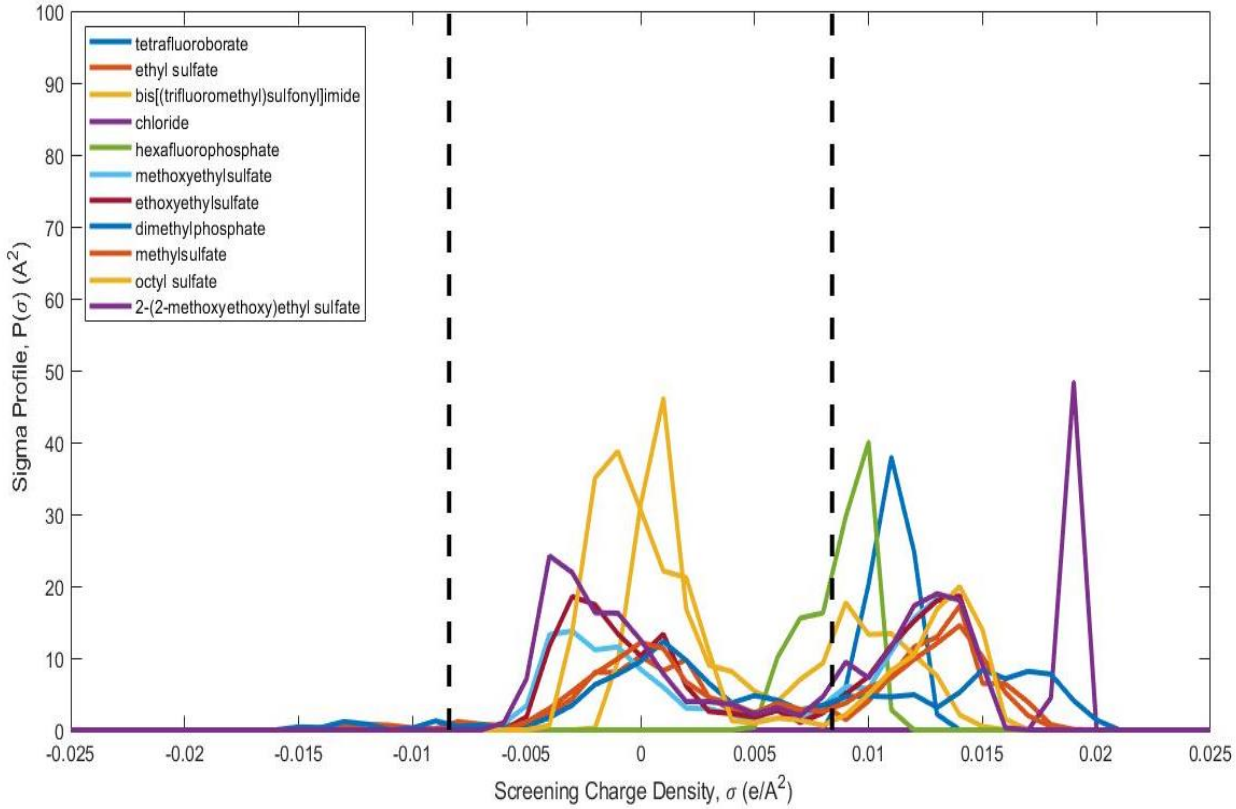


Figure 2: Sigma Profiles of anions used in this work.

4.2 Sigma Profile of Solutes and Polarity

The σ-profiles of solutes are from the VT Sigma Profile Database. They are broadly classified as polar and non-polar. The σ-profiles of some representative polar solutes (Figures 4.3 and 4.4) and non-polar solutes (Figures 4.5 and 4.6) are provided.

Polar compounds generally have portions of their sigma profile in both the hydrogen donor and hydrogen acceptor regions of the σ-profiles. Alcohols (Figure 4.3) have peaks in the non-hydrogen donor region and a small of the σ-profile in the hydrogen donor zone and hydrogen acceptor zone. Water is another example of a polar compound. It has σ-profiles distributed in all the three regions of the sigma profile.

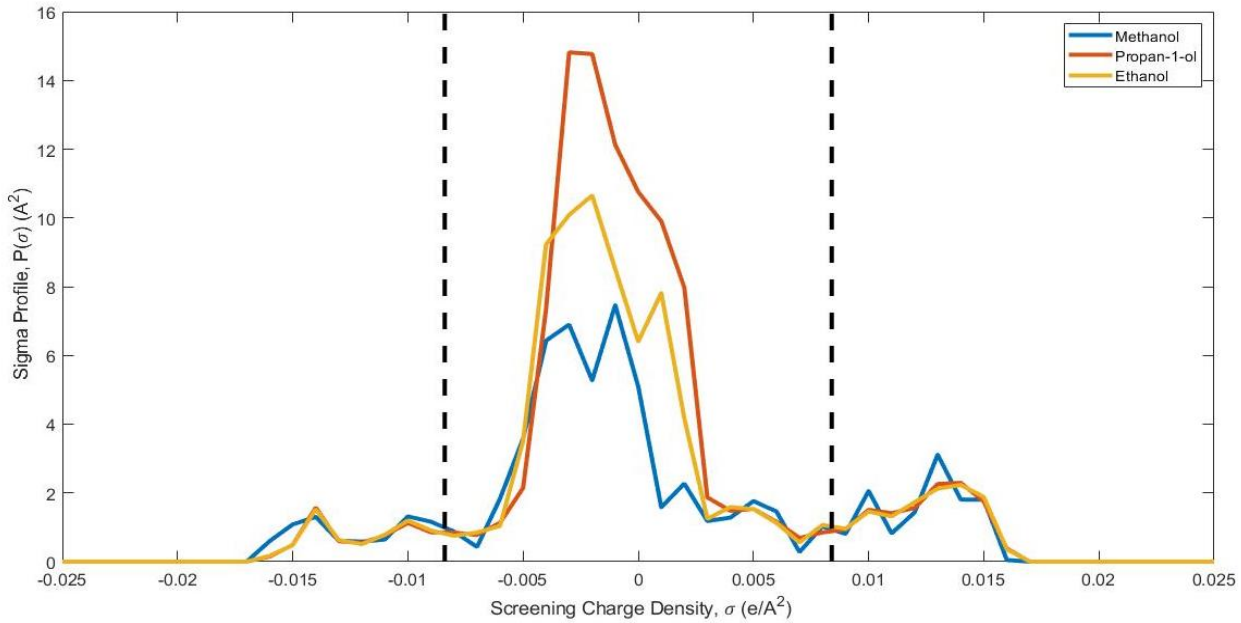


Figure 3: Sigma profiles of alkanols

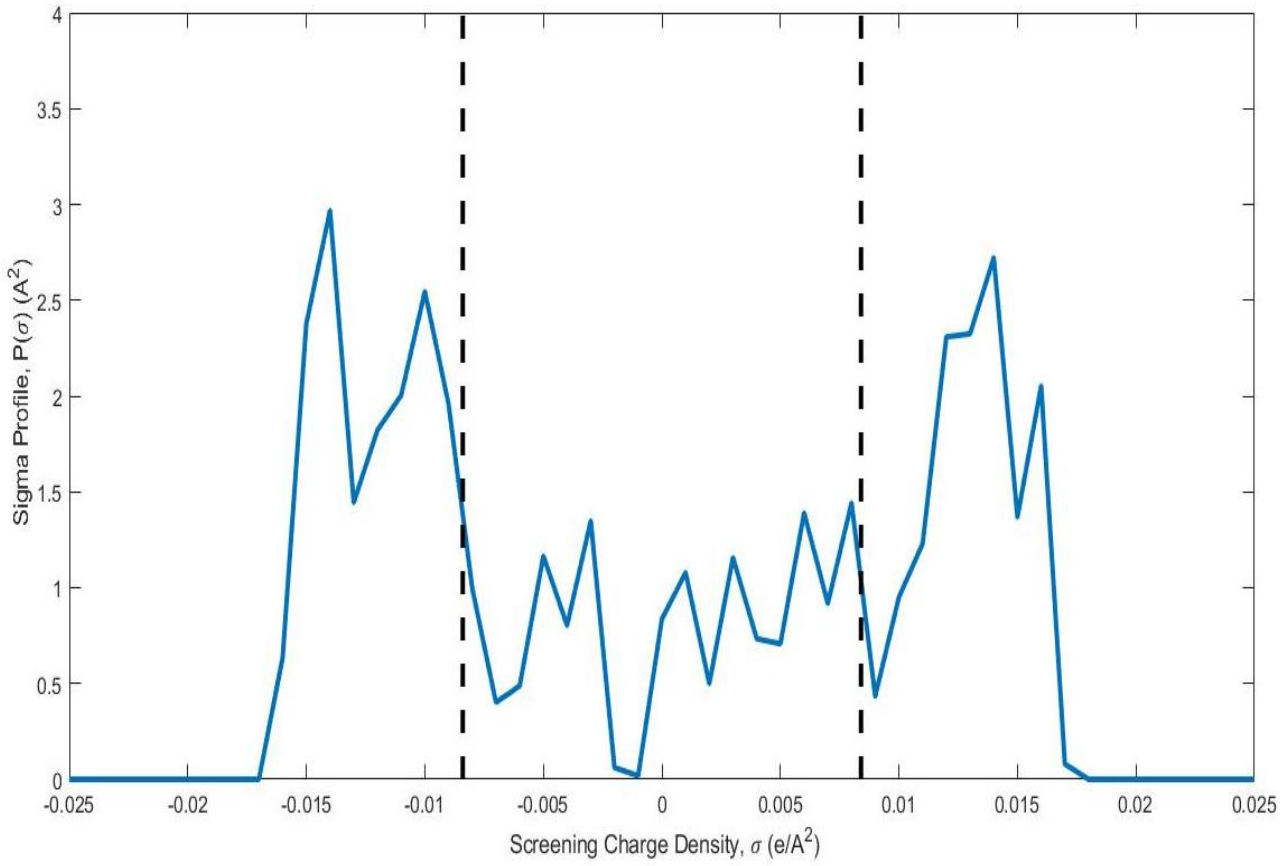


Figure 4: Sigma Profile of water

The σ-profiles of highly non-polar compounds lies almost completely in the non-hydrogen bonding region. Hydrocarbons generally exhibit this kind of σ-profile. For example, 1-heptyne and 1-hexyne in Figure 4.5 have a very small part of the σ-profiles lying in the acceptor and donor regions. 1,3 dimethylbenzene, benzene, styrene and thiophene, all highly non-polar compounds as well, have σ-profiles almost completely in the non-hydrogen bonding region (Figure 4.6).

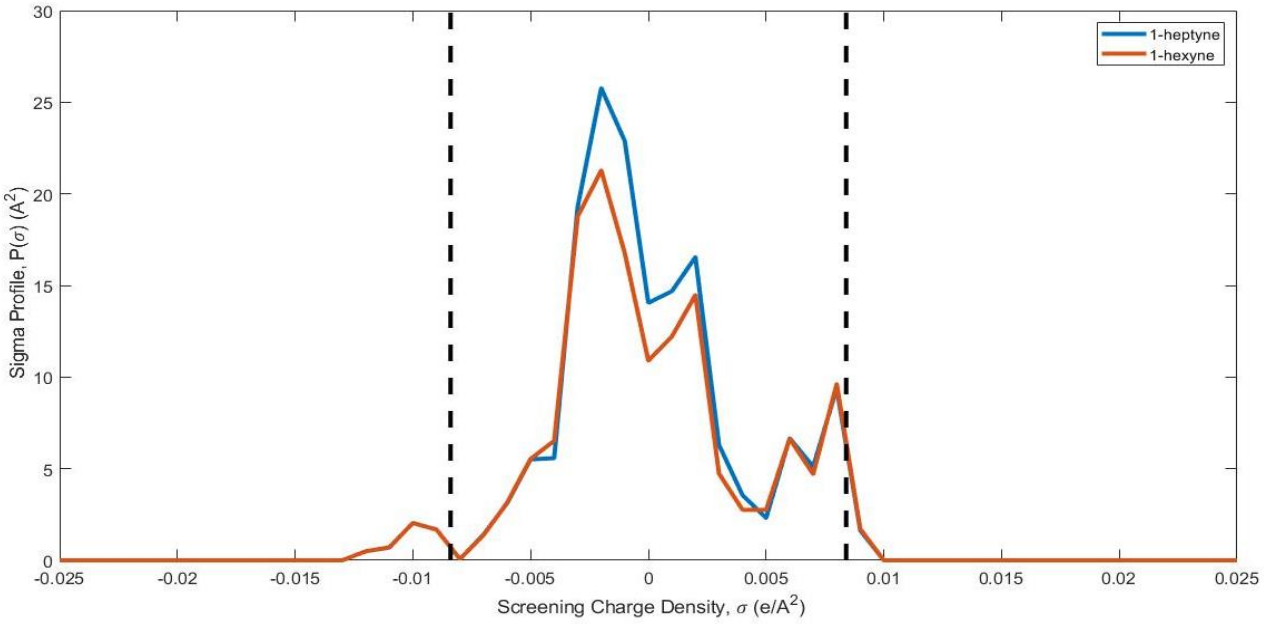


Figure 5: Sigma profiles of 1-heptyne and 1-hexyne

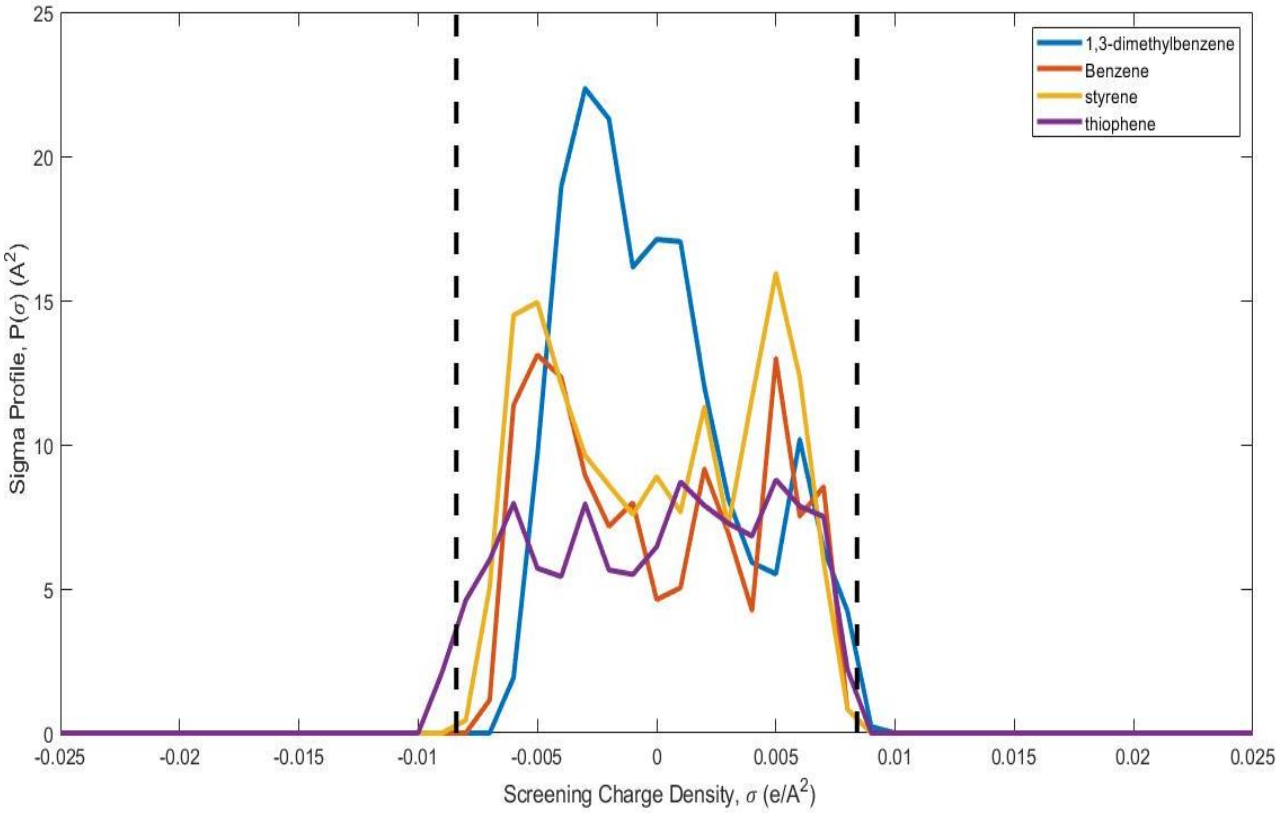


Figure 6: Sigma profiles of Aromatics

4.3 Optimization of Parameters

Figure 4.7 is the parity plot of experimental data to the calculated results using the original COSMO-SAC model. The original COSMO-SAC model gave poor predictions as compared to the experimental values.

The Average Relative Deviation (ARD) of the original model for 414 data points was found to be 6959%. This is mainly because the original COSMO-SAC model parameters were not fitted with experimental data for ionic liquid systems., the need to modify the model became clear if further reduction in ARD was to be expected, hence the modification of the original model.

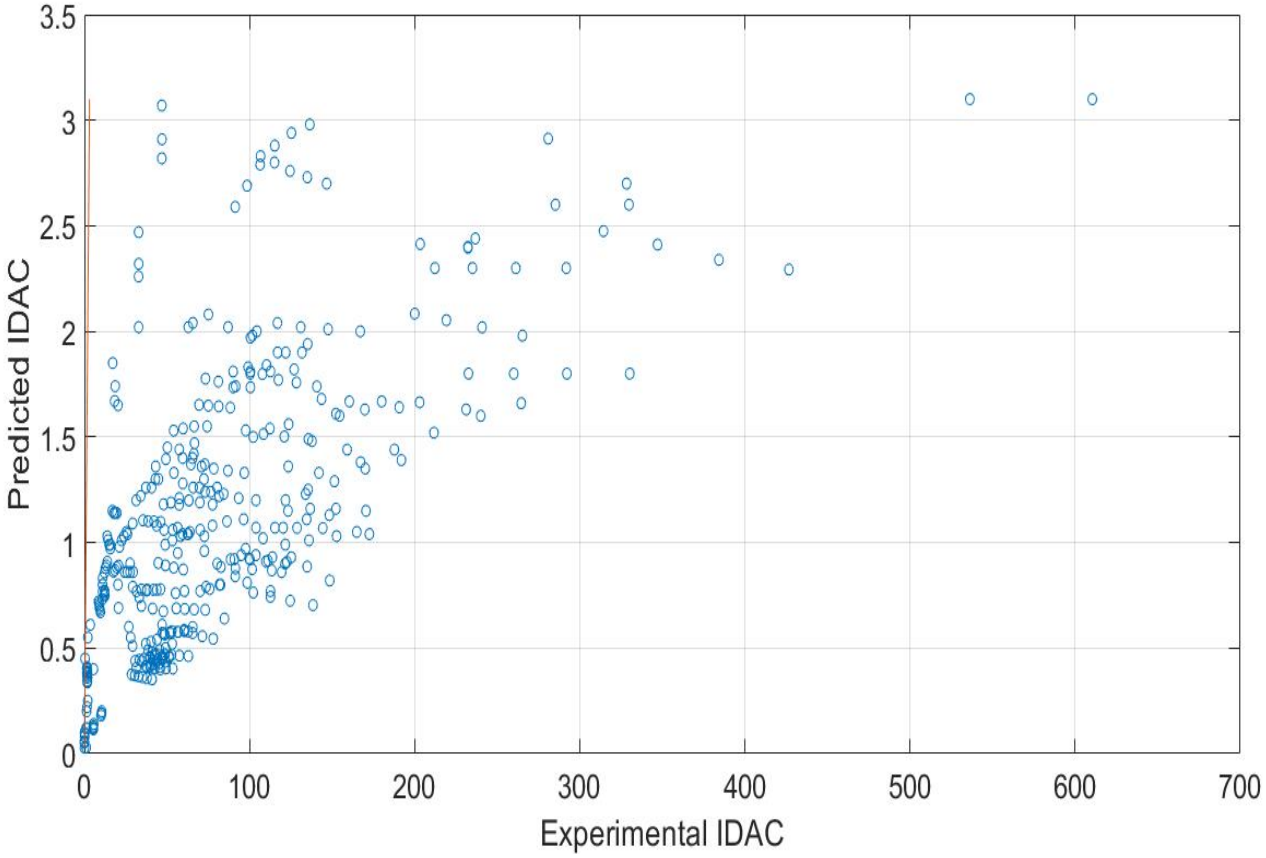


Figure 7: Comparison between experimental data and calculated results by the original COSMO-SAC model

In fitting the modified model, C_{HB} and σ_{HB} were made constants as they did not change after preliminary parameter optimization test runs. Hence, only a_{eff}, q, r, C_1, C_2, and C_{ne} were optimized (Table 4.1). Significant improvements were observed as an ARD of 21% was obtained, as seen in Table 7.

Table 4.1: Optimization of Modified COSMO-SAC Model

Parameters	a_{eff} (Å^2)	C_{HB} (KcalÅ^{4}mole^{-1}e^{-2})	Q (Å^2)	r (Å^3)	σ_{HB} (e/Å)	C_1	C_2	C_{ne}
Initial	7.50	85580	79.53	66.69	8.4×10^{-3}	0.10	1.20	0.10
Optimal	7.65	85580	236.61	3.11	8.4×10^{-3}	3.415×10^{-14}	1.278	5.06×10^{-2}

Table 4.2: Comparison of statistical data for COSMO-SAC models (Original and Modified) for optimization run.

Model	R^2	R^2_{adj}	RMSE	ARD (%)
Original COSMO-SAC	0.024	0.012	0.685	6959
Modified COSMO-SAC	0.916	0.915	0.20	21

Note that the same data points were used in the plots of figures 4.7 and 4.8, with the only difference being that the original parameters of COSMO-SAC 2002 (initial values in Table 6, and without the newly introduced parameters C_1, C_2 and C_{ne}) was used for Figure 4.7, while the optimal parameters in Table 4.1 was used for Figure 4.8. The use of optimized model parameters gotten from the optimization run clearly yields significant improvement. Therefore, the optimal values of a_{eff}, q, r, C_1, C_2, and C_{ne} to be used in the modified model from this work can be found in Table 4.1.

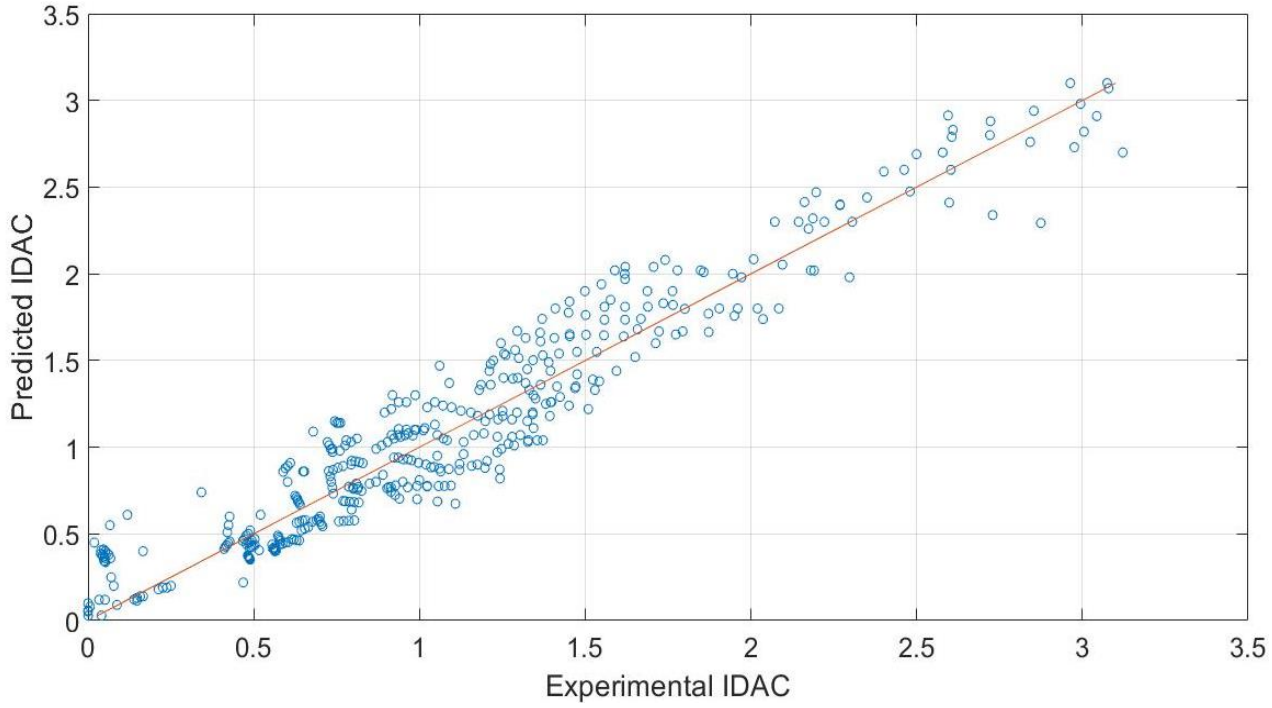


Figure 8: Parity plot for calculated (blue circles) IDAC from the optimized model (Main)

The segment interaction parameters C_1 and C_2 are empirical parameters. C_1 is included in the model to account for the Coulombic Force, which is the sum of electrostatic and van der Waals interactions on ionic liquid. Interestingly, the value of C_1 which is 3.415e-14 is close to the value of coulombic constant for ionic liquids, as proposed by Shi, *et al* (2017). The physical significance of C_2 is unclear, but it serves as a scaling factor for the hydrogen bonding coefficient C_{HB}.

In terms of parameter magnitude, the values of the optimal parameters suggest that the electrostatic term in the model contributes little or is insignificant to this model. The charges on cations and anions of IL are generally delocalized over the surface of the ion. Indeed, it appears to be one of the necessary conditions for ionic liquids that no polarity hotspots are present, since this would lead to aggregation of ions and subsequently to crystallization. (Klamt, (2005)). Thus, for IL systems, it appears that Electrostatic Interaction does not play a major role. However, this will not be the case when the solute is of high polarity, hence the large deviations for solutes with higher polarity.

Non-electrostatic interactions also play a role in the form of long-range intermolecular force. In the original work published by Lin and Sandler (2002), it was assumed that the non-electrostatic interactions cancel out. (Bharti *et al*, 2018) C_{ne} was introduced to test this assumption and evaluate the physical importance of the term. The value of C_{ne} shows that the contribution of the non-electrostatic term is small but does not cancel out.

4.4 ARD Based on Solute Chemical Groups

A closer look at the ARD for the modified model for the various chemical groups indicates that although the ARD for the model is 21%, the ARD of the solutes differs with the chemical group (Figure 4.9). In terms of the lowest ARD, alkynes, nitriles and aromatics have the lowest ARD, while pyridine, alcohol and water had the highest ARD.

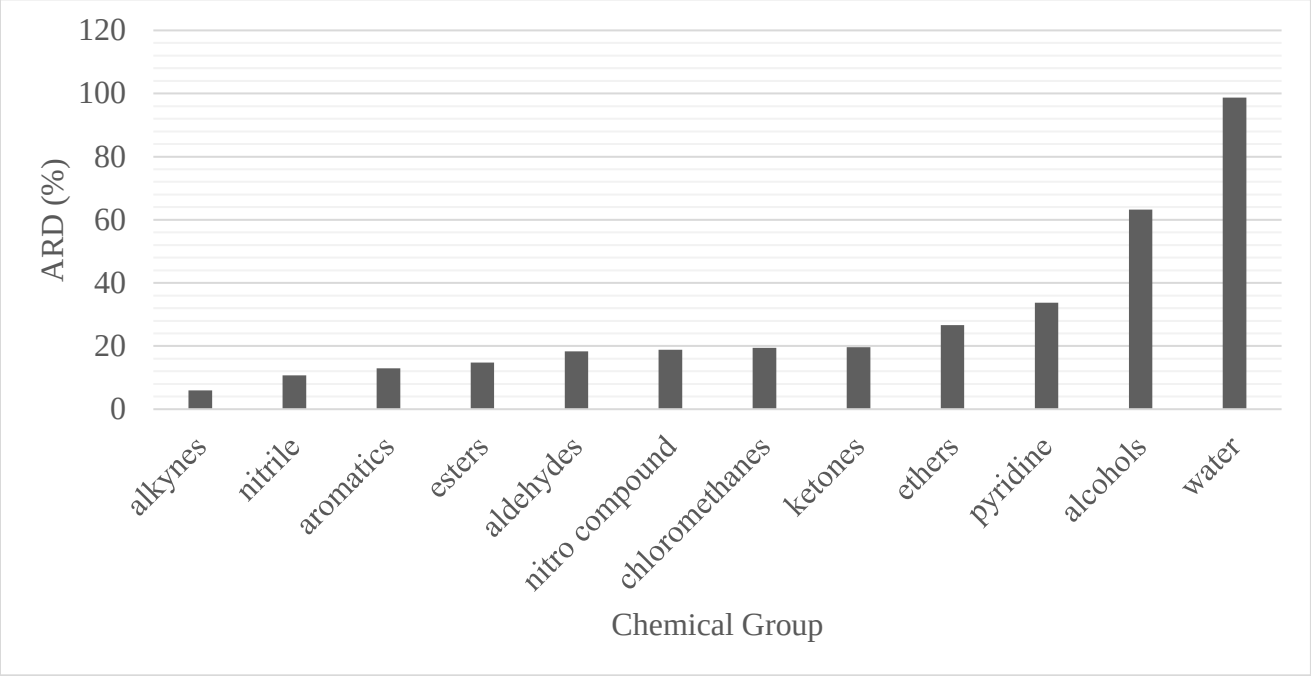


Figure 9: ARD for the various chemical groups used in the curve fitting.

It can be seen from the polarity ranking of organic solutes in Figure 4.10 that the ARD of the different solute groups generally depends on the level of polarity. It appears that solutes with higher polarity have a higher ARD and lower prediction accuracy with this model, while those with lower polarity have a lower ARD and higher prediction accuracy.

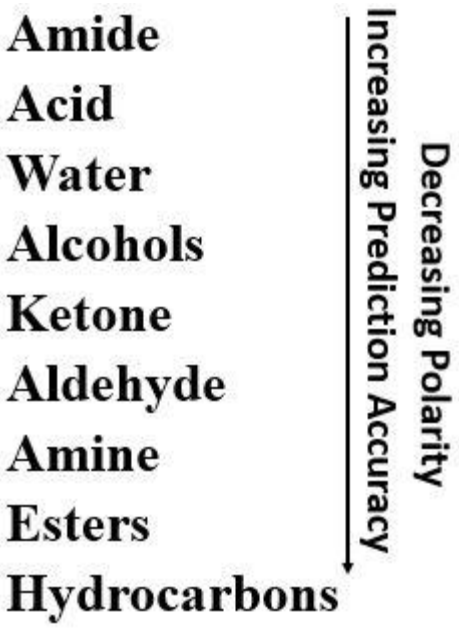


Figure 10: Polarity Ranking and Increasing IDAC Prediction Accuracy

4.5 Validation of The Modified Model

4.5.1 IDAC of new systems

To validate the modified model, the ARD of 29 data points (See Appendix C) which were not included in the parameter optimization, formed using 1 new cation, 1 old cation and 2 new anions (Table 4.3), was computed using the modified model. The ARD value of 18.07% indicates that the model can handle other ionic liquid systems not included in the parameter optimization with a reasonable level of accuracy. For more details on the data points used in the validation, please check the supplementary data file.

Table 4.3: Cations, Anions and Solutes used in the validation of the modified model.

SOLUTES	IL CATIONS	IL ANIONS
ethyl ethanoate	1-butyl-1-methyl-pyrrolidinium	tetracyanoborate
dichloromethane	1-butyl-1-methyl-pyrrolidinium	tetracyanoborate
1,3-dimethylbenzene	1-butyl-1-methyl-pyrrolidinium	tetracyanoborate
Ethylbenzene	1-ethyl-3-methylimidazolium	mesylate
Acetone	1-ethyl-3-methylimidazolium	mesylate
Butanone	1-ethyl-3-methylimidazolium	mesylate
Benzene	1-ethyl-3-methylimidazolium	mesylate

Table 4.4: Comparison of statistical data for COSMO-SAC models (Original and Modified) for validation run.

MODEL	DATA POINTS	R^2	R^2_{adj}	RMSE	ARD (%)
COSMO-SAC (2002)	29	0.3424	0.1630	204.204	6598
Modified COSMO-SAC	29	0.396	0.231	1.569	18.07

4.5.2 Henry's constant

Henry's constant computed using the COSMO-SAC model from this work was compared to experimental values, as well as the values from COSMO-SAC 2010, as reported by Lee and Lin (2015) is shown in Figure 4.11. Although COSMO-SAC 2010 has a different hydrogen bonding model, it was observed that the accuracy of the model from this work was not very far off from that of COSMO-SAC 2010. The COSMO-SAC model from this work has ARD value of 17.2% for 17 data points, as against COSMO-SAC 2010 which has ARD of 9.8%.

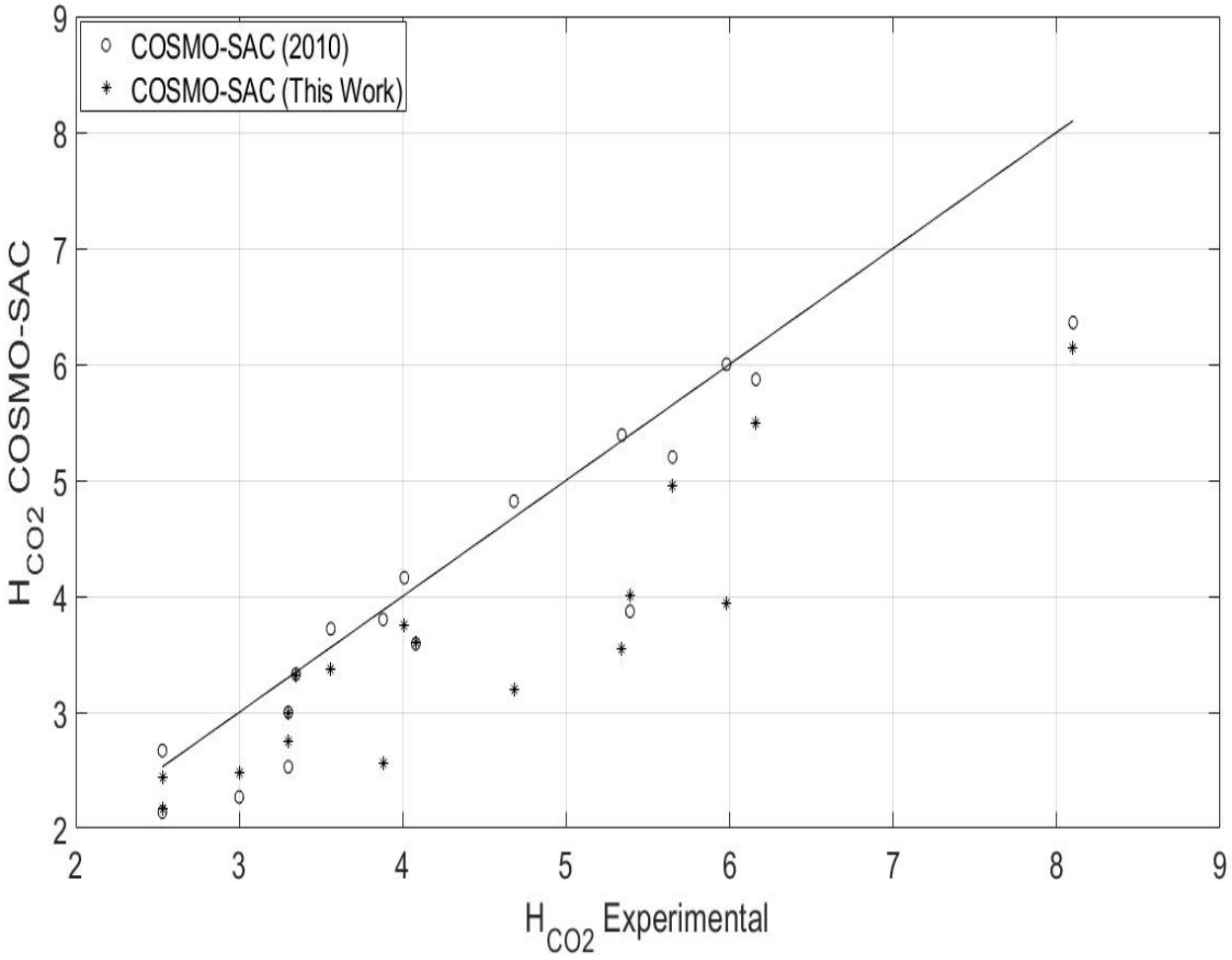


Figure 11: Experimental and COSMO-SAC calculated (this work and COSMO-SAC 2010) plot of Henry's constant.

It is important to note that CO_2 is not among the systems used to fit the new model parameters of the COSMO-SAC model from this work, yet it gives a good Henry's constant prediction for CO_2

in the ionic liquids BMIM-TF_2N and EMIM-TF_2N within the temperature range of 280 to 500K (Figures 4.12 and 4.13). The model performs reasonably well at temperatures below the critical temperature of CO_2, which is 304.15K (31℃). Above the critical temperature the model prediction deviates significantly from the experimental values, as seen in (Figures 4.14 and 4.15). This behaviour tends to agree with the inverse dependency between IDAC and temperature, as described by Krolikowski, *et al* (2021)

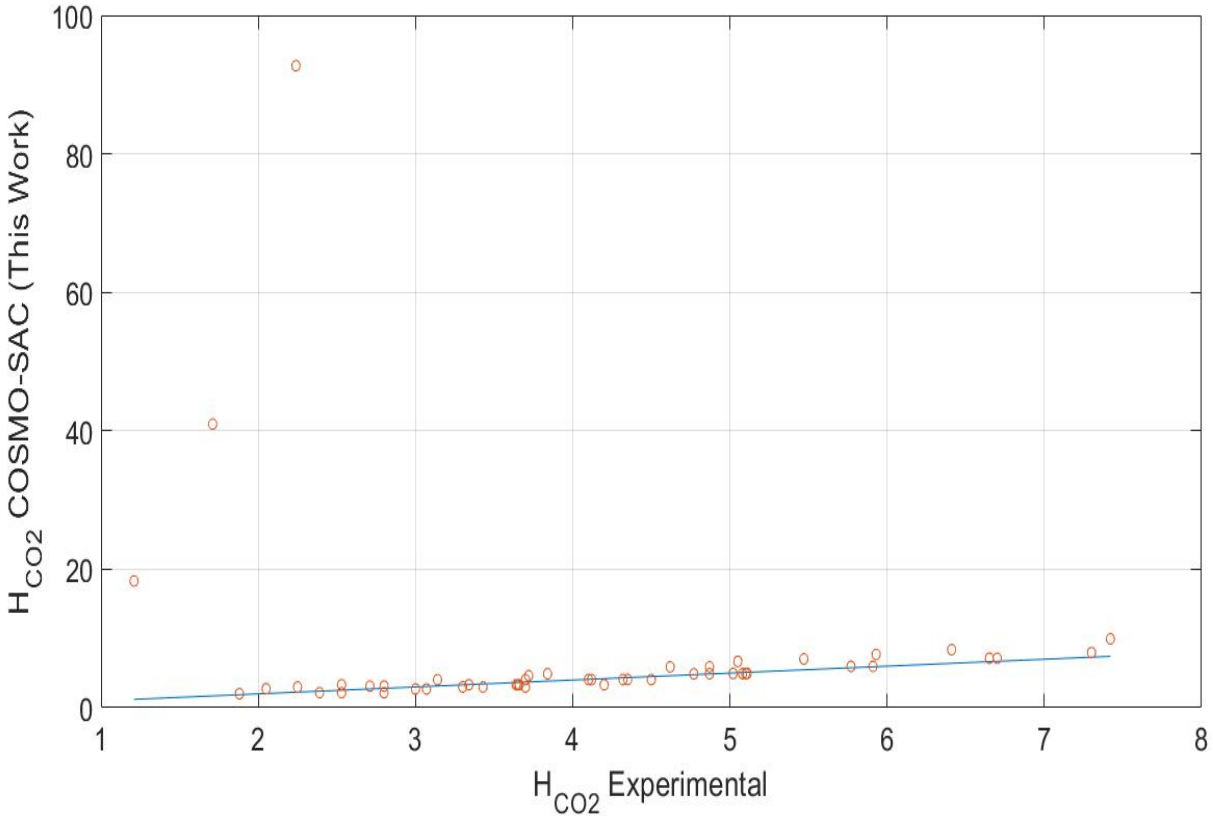


Figure 12: Experimental (blue line) and Calculated (this work, orange circles) Henry's constant for CO_2 in BMIM-TF_2N

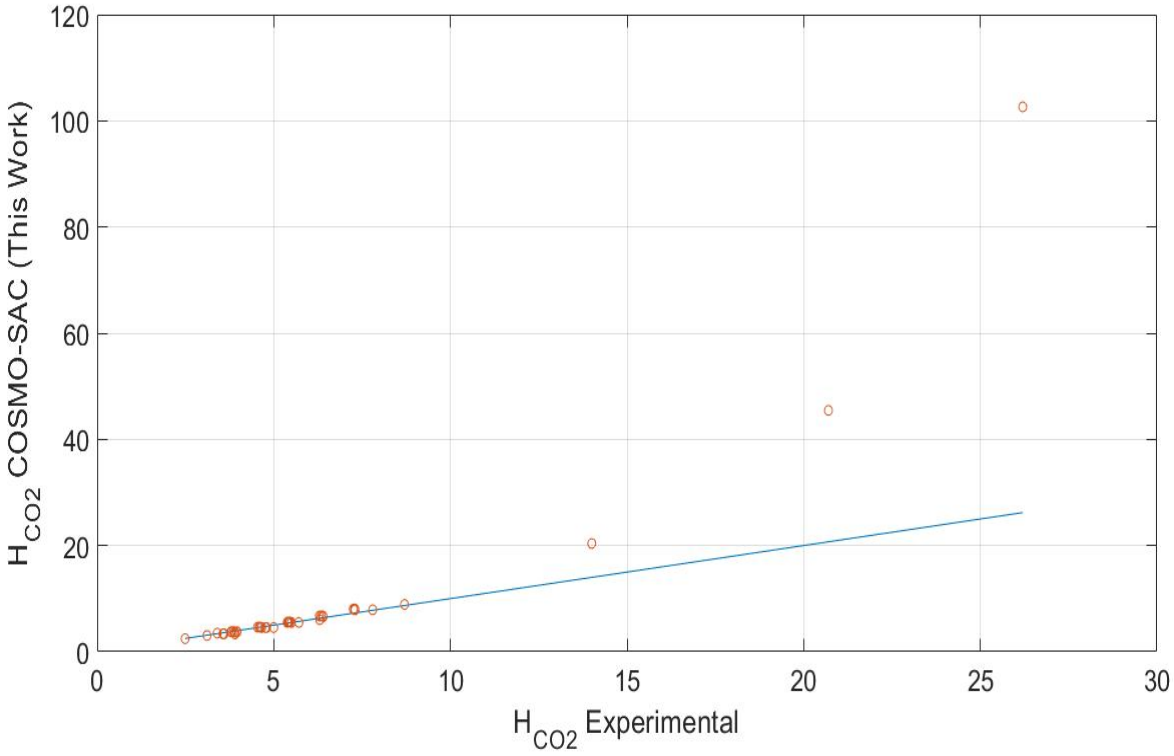


Figure 13:: Experimental (blue line) and Calculated (this work, orange circles) Henry's constant for CO_2 in EMIM-TF_2N

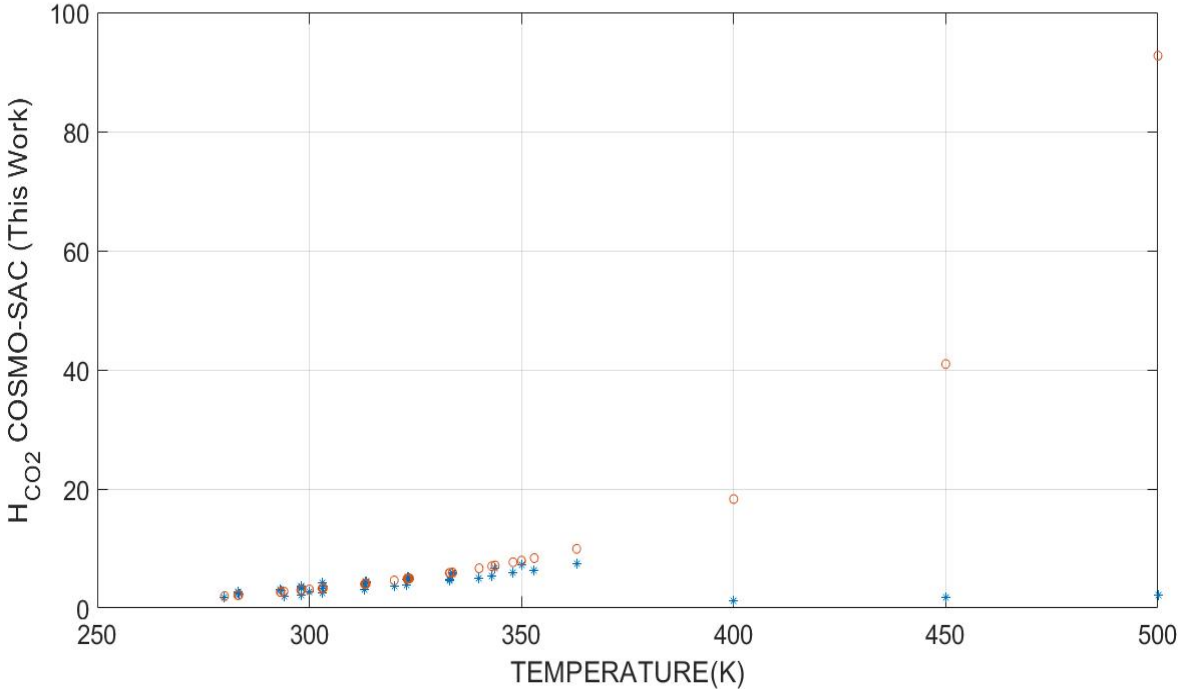


Figure 14: Experimental (blue asterisk) and Calculated (this work, red circles) Henry's constant versus temperature for CO_2 in BMIM-TF_2N

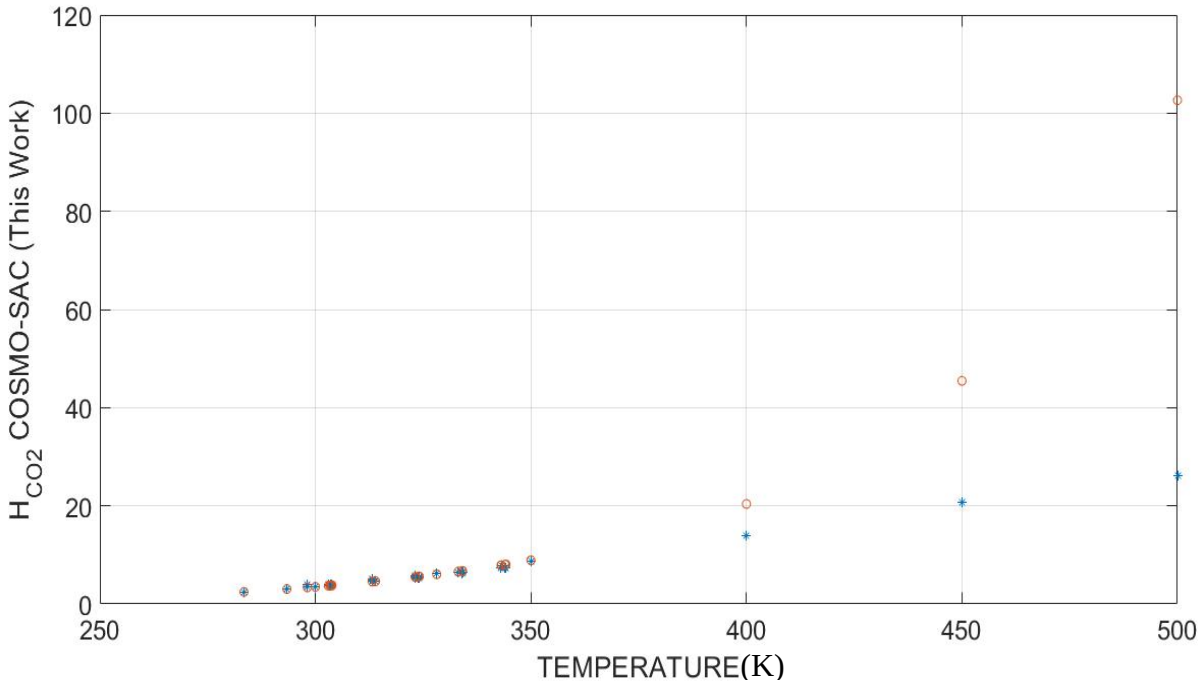


Figure 15: Experimental (blue asterisk) and Calculated (this work, red circles) Henry's constant versus temperature for CO_2 in EMIM-TF_2N

4.5.3 Effect of cation/anion structure on IDAC

To test the effect of alkyl group chain length, four systems were selected, all having benzene as solute, bis[(trifluoromethyl)sulfonyl]imide as anion and 1-Alkyl-3-MethylImidazolium as cation at 313.15K. The alkyl groups on the cation which were studied are methyl, ethyl, butyl and hexyl. It was observed that IDAC of benzene reduced as the alkyl group chain length increased (Figure 4.16). Varying the anions in benzene (1) - 1-Ethyl-3-MethylImidazolium-Anion system at 323.15K also gave a clear variation of IDAC (Figure 4.17). It was noticed that as the IDAC of benzene decreased with increase in branches along the chain length of the anion.

The main reason behind the decrease in IDAC of benzene is the stearic hindrances which hinders access to the core of the molecule, where the chemical interaction should normally take place.

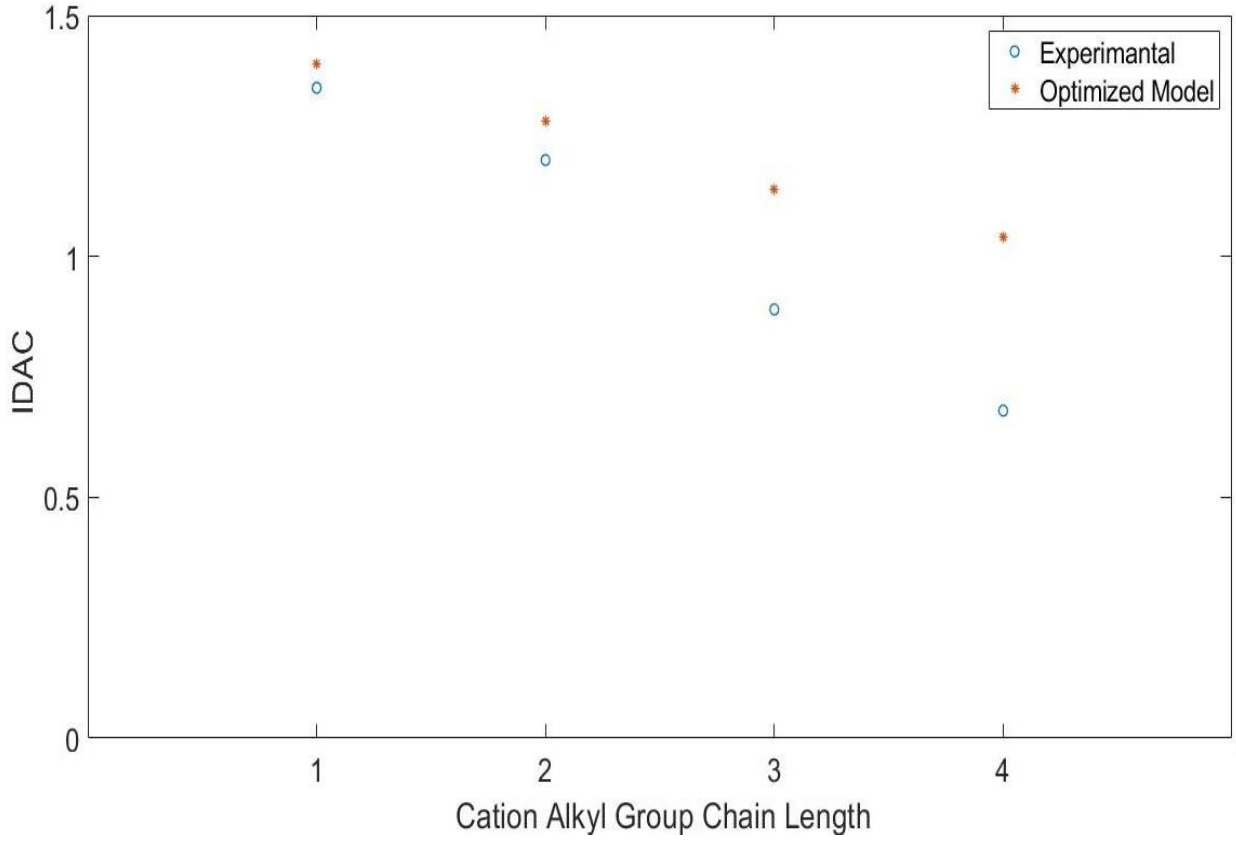


Figure 16: Effect of Alkyl chain length of cation on IDAC of benzene (1) - 1-Alkyl-3-MethylImidazolium bis[(trifluoromethyl)sulfonyl]imide (2) system at 313.15 K from experimental and calculated results

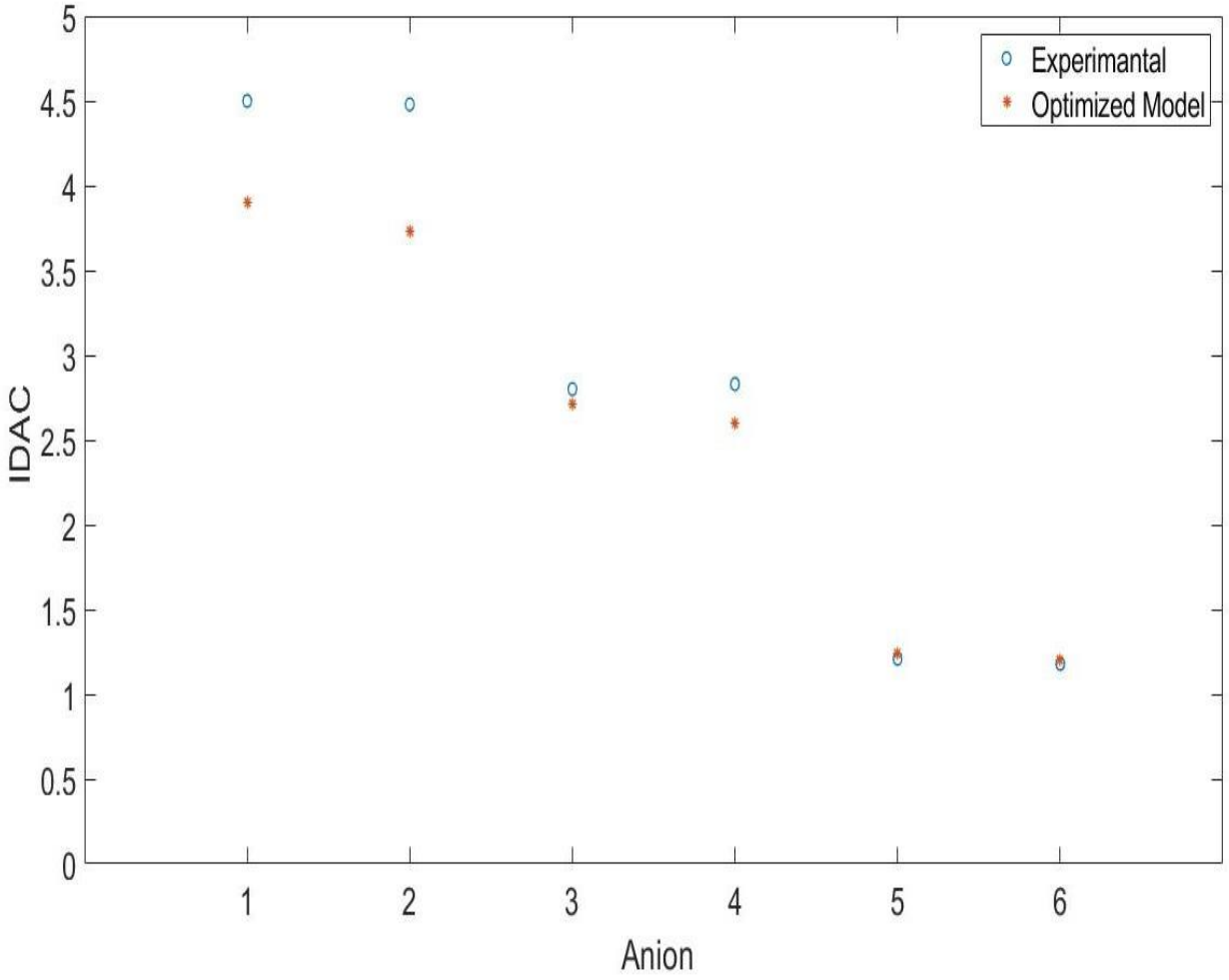


Figure 17: Effect of Anion on IDAC of benzene (1) - 1-Ethyl-3-MethylImidazolium-Anion (2) system at 323.15K from experimental and calculated results.

CHAPTER FIVE

5.0 SUMMARY, CONCLUSION AND RECOMMENDATIONS

5.1 Summary and Conclusion

The COSMO-SAC model was modified by introducing the segment interaction parameters and the non-electrostatic contribution term to the exchange energy expression of the model. The model parameters of the modified model were fitted to experimental data and optimal parameters were obtained. The modified model was further validated and applied to calculating Henry's law constant for CO_2 in ionic liquid and the results compared with COSO-SAC 2010. The following conclusions can be drawn from the study:

I. The Sigma Profiles of 11 Cations, 13 Anions and 10 Solutes that are not in the VT-2005 database have been successfully created.

II. Modifying the adjustable parameters in the exchange energy of the COSMO-SAC model and fitting the model parameters with experimental data improves the accuracy of COSMO-SAC for binary systems of solute in ionic liquid. The optimal values for the parameters a_{eff}, q, and r in the modified model from this works have been determined to be 7.649 Å^2, 236.61 Å^2 and 3.111 Å^3, respectively. Values of C_{HB} and σ_{HB} remain 85580 and 8.4 × 10^{-3} respectively as in the original model. The parameters C_1, C_2 and C_{ne} introduced to the model have been determined to be 3.415 × 10^{-14}, 1.278 and 5.06 × 10^{-2} respectively.

III. The COSMO-SAC model from this work has a lower ARD of 21% as compared to 6959% from the original COSMO-SAC model. Furthermore, validation of the modified model for 29 data points which were not previously used in the parameter optimization yielded an ARD of 18.07 %. This shows that the model can be used for predicting IDAC of ionic

liquid systems not included in the model optimization, especially when the solutes have low polarity. The model has a higher accuracy for solutes that have lower polarity, such as hydrocarbons than for those that have higher polarity like water and alcohols.

IV. The COSMO-SAC model from this work gives a reasonable estimate of Henry's constant for CO_2 in the ionic liquids BMIM-TF_2N and EMIM-TF_2N below the critical temperature of CO_2.

V. The IDAC of benzene in 1-**alkyl**-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide at 313.15K varies with chain length of the alkyl group as follows:

$$\gamma^{\infty}_{Benzene}: \quad \textbf{methyl > ethyl > butyl > hexyl}$$

The IDAC of benzene in 1-ethyl-3-methylimidazolium-**anion** at 323.15K and 333.15K varies with anion type:

$$\gamma^{\infty}_{Benzene}: \quad \textbf{TF2N > EtSO4 > MeSO3}$$

5.2 Recommendations

I. A free web-based sigma profile database for IL cations and anions, like the VT-2005 database for neutral compounds, should be developed in order to ease further works on improving COSMO-based methods for IL systems.

II. Parameter optimization of other versions of COSMO-SAC (2007, 2010, 2013, etc.) for IL systems should be carried out.

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APPENDICES

Refer to CD-ROM attached to inner back cover for complete appendices.

A. Input File for Geometry Optimization and Energy Calculation of a neutral specie

Task parameters

Calculate energy

Basis_version v4.0.0

Electronic parameters

Spin_polarization restricted

Charge 0.0000

Basis dnp

Atom_rcut 5.5000 angstrom

Pseudopotential none

Functional vwn-bp

Aux_density octupole

Integration_grid fine

Scf_density_convergence 1.0000e-006

Scf_charge_mixing 0.2000

Scf_iterations 50

Scf_diis 6 pulay

Occupation fermi

Environment Keywords

Cosmo on

Cosmo_Grid_Size 1082

Cosmo_Segments 92

Cosmo_Solvent_Radius 1.300000

Cosmo_A-Matrix_Cutoff 7.000000

Cosmo_Radius_Incr 0.000000

Cosmo_A-Constant 1.882190

Cosmo_B-Constant 0.010140

Cosmo_RadCorr_Incr 0.150000

Cosmo_Atomic_Radii

1 1.300

6 2.000

7 1.830

8 1.720

9 1.720

15 2.120

16 2.160

17 2.050

35 2.160

53 2.320

Print options

Print eigval_last_it

Calculated properties

B. Supplementary Data for Parameter Optimization

Table B.1: Abbreviations, names and structures of cations and anions

CATIONS					ANIONS				
S.No.	**Abbreviations**	**Names**	**Formula**	**Computation ID. No**	**S.No.**	**Abbreviations**	**Names**	**Formula**	**Computation ID. No**
1	[BMIM]	1-butyl-3-methyl-imidazolium	$C_8H_{15}N_2$	63	1	[BF_4]	tetrafluoro borate	BF_4	70
2	[BMPY]	1-butyl-4-methyl-pyridinium	$C_{10}H_{16}N$	58	2	[Cl]	chloride	Cl	73
3	[BMPYR]	1-butyl-1-methyl-pyrrolidinium	$C_9H_{20}N$	699	3	[$DMPO_4$]	dimethylp hosphate	$C_2H_6O_4P$	77
4	[EMIM]	1-ethyl-3-methyl-imidazolium	$C_6H_{11}N_2$	59	4	[$EtSO_4$]	ethyl sulfate	C_2H5O4S	71
5	[EPY]	ethylpyridiniu m	$C_7H_{10}N$	69	5	[$MeSO_3$]	Methanesu lfonate (mesylate)	CH3O3S	845
6	[HMIM]	1-hexyl-3-methyl-imidazolium	$C_{10}H_{19}N_2$	66	6	[$MeSO_4$]	methyl sulfate	CH3O4S	78
7	[MMIM]	1,3-dimethyl-imidazolium	$C_5H_9N_2$	60	7	[PF_6]	hexafluoro phosphate	F6P	74
8	[$N_{4,1,1,1}$]	*N,N,N,N*-trimethylbutyl ammonium	$C_7H_{18}N$	64	8	[TCB]	tetracyano borate	C4BN4	850
9	[OMIM]	1-octyl-3-methyl-imidazolium	$C_{12}H_{23}N_2$	65	9	[Tf_2N]	bis(trifluor omethylsul fonyl)-amide	C2F6NO4S2	72
10	[EMMIM]	1-ethyl-2,3-dimethylimid azolium	$C_7H_{13}N_2$	62	10	[C8SO4]	Octylsulfat e	C8H17O4S	80
11	[PY]	Pyridinium	C_5H_6N	68	11	[$MOEtSO_4$]	methoxyet hylsulfate	C3H7O5S	75
					12	[MDEGS O_4]	2-(2-Methoxyet hoxy)ethyl sulfate	C5H11O6S	81
					13	[$C_2H_5OC_2$ H_4OSO_3]	ethoxyethy lsulfate	C9H15NO5S	76

Table B.2: Activity coefficients at infinite dilution of organic compounds dissolved in ionic liquids.

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
1		58	70	94	313.15	1.639	44.18	1.62	25.96	0.01	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2001) J. Chem. Eng. Data 46(6), 1526-1529
2		58	70	94	323.15	1.645	40.67	1.56	23.72	0.05	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2001) J. Chem. Eng. Data 46(6), 1526-1529
3		58	70	94	333.15	1.648	37.53	1.50	21.77	0.09	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2001) J. Chem. Eng. Data 46(6), 1526-1529
4		58	70	94	343.15	1.652	34.72	1.45	20.02	0.12	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2001) J. Chem. Eng. Data 46(6), 1526-1529
5		58	70	96	313.15	1.98	132.6	2.30	65.99	0.16	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2001) J. Chem. Eng. Data 46(6), 1526-1529
6		58	70	96	323.15	2.019	120.4	2.19	58.64	0.09	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2001) J. Chem. Eng. Data 46(6), 1526-1529
7		58	70	96	333.15	2.053	109.6	2.09	52.39	0.02	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2001) J. Chem. Eng. Data 46(6), 1526-1529
8		58	70	96	343.15	2.084	100	2.01	46.99	0.04	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2001) J. Chem. Eng. Data 46(6), 1526-1529
9		60	72	94	293.15	1.33	48.41	1.53	35.40	0.15	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
10		60	72	94	303.15	1.34	43.45	1.47	31.43	0.10	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417

Data	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC	RD (This Work)	Experimental method	Reference
11		60	72	94	313.15	1.35	39.18	1.41	28.02	0.05	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
12		60	72	94	323.15	1.36	35.48	1.37	25.09	0.00	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
13		60	72	94	333.15	1.37	32.25	1.32	22.54	0.04	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
14		60	72	93	293.15	2	83.52	1.95	40.76	0.03	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
15		60	72	93	303.15	2.01	73.78	1.86	35.71	0.08	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
16		60	72	93	313.15	2.02	65.52	1.78	31.44	0.12	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
17		60	72	93	323.15	2.04	58.46	1.71	27.66	0.16	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
18		59	71	94	293.15	2.7	73.35	3.12	26.17	0.16	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
19		59	71	94	303.15	2.73	67.49	2.98	23.72	0.09	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
20		59	71	94	313.15	2.76	62.26	2.84	21.56	0.03	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC	RD (This Work)	Experimental method	Reference
21		59	71	94	323.15	2.8	57.57	2.72	19.56	0.03	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
22		59	71	94	333.15	2.83	53.34	2.61	17.85	0.08	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
23		58	70	19	313.76	0.908	61.29	0.83	66.50	0.09	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
24		58	70	19	323.02	0.914	55.6	0.82	59.83	0.11	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
25		58	70	19	333.25	0.919	50.15	0.81	53.57	0.12	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
26		58	70	19	343.58	0.921	45.4	0.80	48.29	0.14	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
27		58	70	22	313.71	0.58	30.2	0.66	51.08	0.13	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
28		58	70	22	322.93	0.577	28.19	0.65	47.86	0.12	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
29		58	70	22	333.23	0.57	26.18	0.64	44.93	0.12	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
30		58	70	22	343.57	0.564	24.38	0.63	42.23	0.12	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
31		58	70	32	313.68	0.748	6.199	0.83	7.29	0.10	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
32		58	70	32	323.02	0.757	6.186	0.81	7.17	0.07	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
33		58	70	32	333.38	0.766	6.154	0.80	7.03	0.04	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
34		58	70	32	343.78	0.772	6.106	0.79	6.91	0.02	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
35		58	70	33	313.73	0.732	5.42	0.74	6.40	0.01	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
36		58	70	33	323.05	0.768	5.471	0.74	6.12	0.04	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
37		58	70	33	333.46	0.8	5.507	0.73	5.88	0.08	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
38		58	70	33	343.96	0.832	5.521	0.73	5.64	0.12	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Thermodyn. 34(8), 1341-1347
39		59	72	33	313.15	0.972	7.827	0.74	7.05	0.24	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
40		59	72	33	323.15	0.989	7.502	0.73	6.59	0.26	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC	RD (This Work)	Experimental method	Reference
41		59	72	33	333.15	1.011	7.193	0.73	6.11	0.28	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
42		59	72	33	343.15	1.029	6.9	0.72	5.71	0.30	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
43		59	72	32	313.15	0.891	10.32	0.77	10.59	0.14	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
44		59	72	32	323.15	0.882	9.771	0.75	10.08	0.15	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
45		59	72	32	333.15	0.869	9.26	0.74	9.66	0.15	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
46		59	72	32	343.15	0.862	8.787	0.73	9.19	0.16	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
47		59	72	18	313.15	0.886	67.46	1.04	75.14	0.18	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
48		59	72	18	323.15	0.9	60.75	1.02	66.50	0.13	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
49		59	72	18	333.15	0.91	54.94	1.00	59.38	0.10	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
50		59	72	18	343.15	0.924	49.89	0.98	52.99	0.06	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
51		59	72	19	313.15	0.399	22.94	0.56	56.49	0.41	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
52		59	72	19	323.15	0.406	21.33	0.56	51.53	0.38	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
53		59	72	19	333.15	0.412	19.88	0.56	47.26	0.36	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
54		59	72	19	343.15	0.415	18.58	0.56	43.78	0.34	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
55		59	72	22	313.15	0.435	24.42	0.50	55.14	0.16	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
56		59	72	22	323.15	0.429	22.76	0.50	52.06	0.16	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
57		59	72	22	333.15	0.425	21.27	0.49	49.05	0.16	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
58		59	72	22	343.15	0.419	19.93	0.49	46.56	0.16	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
59		59	72	91	313.15	2.396	116.1	2.27	47.47	0.05	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
60		59	72	91	323.15	2.414	101.7	2.16	41.12	0.10	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899

Data Point	IL - Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
61	59	72	93	313.15	1.735	50.26	1.62	27.97	0.07	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
62	59	72	93	323.15	1.735	45.05	1.56	24.96	0.10	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
63	59	72	93	333.15	1.762	40.56	1.50	22.02	0.15	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
64	59	72	93	343.15	1.776	36.67	1.45	19.65	0.18	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
65	59	72	94	313.15	1.199	31.61	1.29	25.37	0.08	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
66	59	72	94	323.15	1.179	28.72	1.25	23.36	0.06	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
67	59	72	94	333.15	1.189	26.19	1.21	21.02	0.02	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
68	59	72	94	343.15	1.181	23.97	1.18	19.29	0.00	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
69	59	72	96	313.15	1.664	101.5	1.87	60.00	0.13	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
70	59	72	96	323.15	1.668	90.02	1.79	52.97	0.08	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
71		59	72	96	333.15	1.668	80.22	1.72	47.09	0.03	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
72		59	72	96	343.15	1.68	71.81	1.66	41.74	0.01	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
73		62	72	19	313.15	0.462	31.47	0.64	67.12	0.38	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
74		62	72	19	323.15	0.464	28.76	0.63	60.98	0.36	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
75		62	72	19	333.15	0.468	26.38	0.62	55.37	0.33	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
76		62	72	19	343.15	0.469	24.28	0.61	50.78	0.31	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
77		62	72	22	313.15	0.462	25.67	0.49	54.56	0.07	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
78		62	72	22	323.15	0.453	23.86	0.49	51.67	0.08	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
79		62	72	22	333.15	0.449	22.24	0.48	48.54	0.08	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
80		62	72	22	343.15	0.44	20.79	0.48	46.25	0.09	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
81		62	72	32	313.15	0.909	6.919	0.61	6.61	0.33	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
82		62	72	32	323.15	0.892	6.631	0.60	6.43	0.32	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
83		62	72	32	333.15	0.879	6.36	0.60	6.23	0.32	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
84		62	72	32	343.15	0.858	6.103	0.59	6.11	0.31	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
85		62	72	18	313.15	1.068	72.19	0.98	66.59	0.08	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
86		62	72	18	323.15	1.069	64.37	0.96	59.22	0.11	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
87		62	72	18	333.15	1.07	57.69	0.94	52.92	0.13	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
88		62	72	18	343.15	1.07	51.95	0.92	47.55	0.14	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
89		62	72	94	313.15	1.097	23.09	1.01	20.05	0.08	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
90		62	72	94	323.15	1.1	21.06	0.98	18.15	0.10	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
91		62	72	94	333.15	1.101	19.28	0.96	16.52	0.13	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
92		62	72	94	343.15	1.105	17.72	0.94	15.04	0.15	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
93		62	72	96	313.15	1.49	67.82	1.39	44.52	0.07	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
94		62	72	96	323.15	1.502	60.5	1.34	39.28	0.11	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
95		62	72	96	333.15	1.514	54.23	1.30	34.82	0.14	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
96		62	72	96	343.15	1.531	48.82	1.26	30.89	0.18	Gas–Liquid Chromatography	Heintz, A.; Kulikov, D. V.; Verevkin, S. P. (2002) J. Chem. Eng. Data 47(4), 894-899
97		59	72	38	293.15	0.703	69.21	0.94	97.45	0.34	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
98		59	72	38	303.15	0.724	62.32	0.93	85.07	0.28	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
99		59	72	38	313.15	0.743	56.34	0.91	74.83	0.23	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
100		59	72	38	323.15	0.763	51.14	0.90	66.02	0.18	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
101		59	72	39	293.15	0.544	39.01	0.71	70.71	0.30	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
102		59	72	39	303.15	0.556	35.71	0.70	63.23	0.27	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
103		59	72	39	313.15	0.571	32.8	0.70	56.44	0.23	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
104		59	72	39	323.15	0.586	30.22	0.70	50.57	0.19	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
105		59	72	19	293.15	0.403	26.76	0.57	65.41	0.41	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
106		59	72	19	303.15	0.404	24.74	0.57	60.24	0.40	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
107		59	72	19	313.15	0.41	22.94	0.56	54.95	0.38	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
108		59	72	19	323.15	0.423	21.33	0.56	49.42	0.33	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
109		59	72	93	293.15	1.82	63.51	1.76	33.89	0.03	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
110		59	72	93	303.15	1.81	56.35	1.69	30.13	0.07	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
111		59	72	93	313.15	1.81	50.26	1.62	26.77	0.10	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
112		59	72	93	323.15	1.81	45.05	1.56	23.89	0.14	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
113		59	72	94	293.15	1.18	38.81	1.39	31.89	0.18	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
114		59	72	94	303.15	1.19	34.95	1.34	28.37	0.13	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
115		59	72	94	313.15	1.2	31.61	1.29	25.34	0.08	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
116		59	72	94	323.15	1.21	28.72	1.25	22.73	0.03	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
117		63	72	94	293.15	0.872	29.94	1.24	33.34	0.42	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
118		63	72	94	303.15	0.881	27.04	1.20	29.70	0.36	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
119		63	72	94	313.15	0.892	24.54	1.16	26.51	0.30	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
120		63	72	94	323.15	0.903	22.36	1.12	23.76	0.24	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417

Data Point	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
121	63	72	93	303.15	1.22	40.79	1.51	32.43	0.24	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
122	63	72	93	313.15	1.24	36.57	1.45	28.49	0.17	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
123	63	72	93	323.15	1.26	32.94	1.40	25.14	0.11	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
124	63	72	93	333.15	1.28	29.81	1.35	22.29	0.05	The Dilutor Technique	Krummen, M.; Wasserscheid, P.; Gmehling, J. (2002) J. Chem. Eng. Data 47(6), 1411-1417
125	65	73	45	298.15	3.07	23.45	3.08	6.64	0.00	Gas–Liquid Chromatography	David, W.; Letcher, T. M.; Ramjugernath, D.; Raal, J. D. (2003) J. Chem. Thermodyn. 35(8), 1335-1341
126	65	73	45	308.15	2.91	23.49	3.04	7.07	0.05	Gas–Liquid Chromatography	David, W.; Letcher, T. M.; Ramjugernath, D.; Raal, J. D. (2003) J. Chem. Thermodyn. 35(8), 1335-1341
127	65	73	45	318.15	2.82	23.44	3.00	7.31	0.07	Gas–Liquid Chromatography	David, W.; Letcher, T. M.; Ramjugernath, D.; Raal, J. D. (2003) J. Chem. Thermodyn. 35(8), 1335-1341
128	65	73	47	298.15	2.47	16.42	2.20	5.65	0.11	Gas–Liquid Chromatography	David, W.; Letcher, T. M.; Ramjugernath, D.; Raal, J. D. (2003) J. Chem. Thermodyn. 35(8), 1335-1341
129	65	73	47	308.15	2.32	16.43	2.19	6.08	0.06	Gas–Liquid Chromatography	David, W.; Letcher, T. M.; Ramjugernath, D.; Raal, J. D. (2003) J. Chem. Thermodyn. 35(8), 1335-1341
130	65	73	47	318.15	2.26	16.4	2.17	6.25	0.04	Gas–Liquid Chromatography	David, W.; Letcher, T. M.; Ramjugernath, D.; Raal, J. D. (2003) J. Chem. Thermodyn. 35(8), 1335-1341

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
131		66	74	94	298.15	1.03	36.32	1.13	34.27	0.10	Gas–Liquid Chromatography	Letcher, T. M.; Soko, B.; Ramjugernath, D.; Deenadayalu, N.; Nevines, A.; Naicker, P. K. (2003) J. Chem. Eng. Data 48(3), 708-711
132		66	74	94	313.15	1.04	31.14	1.08	28.94	0.04	Gas–Liquid Chromatography	Letcher, T. M.; Soko, B.; Ramjugernath, D.; Deenadayalu, N.; Nevines, A.; Naicker, P. K. (2003) J. Chem. Eng. Data 48(3), 708-711
133		66	74	94	323.15	1.07	28.24	1.05	25.39	0.02	Gas–Liquid Chromatography	Letcher, T. M.; Soko, B.; Ramjugernath, D.; Deenadayalu, N.; Nevines, A.; Naicker, P. K. (2003) J. Chem. Eng. Data 48(3), 708-711
134		66	74	94	298.15	0.96	36.32	1.13	36.84	0.18	Gas–Liquid Chromatography	Letcher, T. M.; Soko, B.; Ramjugernath, D.; Deenadayalu, N.; Nevines, A.; Naicker, P. K. (2003) J. Chem. Eng. Data 48(3), 708-711
135		66	74	94	323.15	0.95	28.24	1.05	28.73	0.11	Gas–Liquid Chromatography	Letcher, T. M.; Soko, B.; Ramjugernath, D.; Deenadayalu, N.; Nevines, A.; Naicker, P. K. (2003) J. Chem. Eng. Data 48(3), 708-711
136		66	74	27	323.15	0.61	1.767	0.12	1.90	0.81	Gas–Liquid Chromatography	Letcher, T. M.; Soko, B.; Reddy, P.; Deenadayalu, N. (2003) J. Chem. Eng. Data 48(6), 1587-1590
137		60	77	29	343.15	0.18	5.027	0.21	26.93	0.18	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
138		60	77	29	353.15	0.19	5.115	0.23	25.92	0.19	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
139		60	77	29	363.15	0.19	5.19	0.24	26.31	0.25	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
140		60	77	29	373.15	0.2	5.251	0.25	25.25	0.25	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
141		60	77	30	343.15	0.122	2.659	0.14	20.79	0.14	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
142		60	77	30	353.15	0.13	2.72	0.15	19.92	0.14	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
143		60	77	30	363.15	0.14	2.775	0.16	18.82	0.12	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
144		60	77	30	373.15	0.14	2.823	0.17	19.16	0.19	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
145		60	77	19	303.15	2.3	145.9	2.31	62.44	0.00	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
146		60	77	19	313.15	2.3	130.6	2.22	55.80	0.03	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
147		60	77	19	323.15	2.3	117.5	2.14	50.09	0.07	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
148		60	77	19	333.15	2.3	106.1	2.07	45.14	0.10	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
149		60	78	27	333.15	0.55	1.053	0.07	0.91	0.88	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
150		69	72	54	303.15	1.15	85.25	1.33	73.13	0.15	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
151		69	72	54	313.15	1.16	76.18	1.28	64.67	0.10	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
152		69	72	54	323.15	1.16	68.39	1.24	57.95	0.07	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
153		69	72	54	333.15	1.15	61.66	1.20	52.61	0.04	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
154		69	72	38	303.15	0.93	62.64	0.97	66.35	0.04	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
155		69	72	38	313.15	0.93	56.93	0.95	60.21	0.02	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
156		69	72	38	323.15	0.94	51.9	0.94	54.22	0.00	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
157		69	72	38	333.15	0.94	47.47	0.92	49.50	0.02	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
158		69	72	19	303.15	0.46	23.59	0.58	50.29	0.26	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
159		69	72	19	313.15	0.47	22.01	0.58	45.83	0.23	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
160		69	72	19	323.15	0.48	20.58	0.58	41.87	0.20	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
161		69	72	19	333.15	0.49	19.28	0.57	38.35	0.17	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
162		69	72	33	303.15	1.14	9.809	0.76	7.60	0.33	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
163		69	72	33	313.15	1.14	9.332	0.76	7.19	0.34	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
164		69	72	33	323.15	1.14	8.885	0.75	6.79	0.34	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
165		69	72	33	333.15	1.15	8.465	0.74	6.36	0.35	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
166		69	72	32	303.15	1.05	12.76	0.81	11.15	0.23	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
167		69	72	32	313.15	1.03	11.97	0.79	10.62	0.23	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
168		69	72	32	323.15	1.01	11.25	0.78	10.14	0.23	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
169		69	72	32	333.15	0.98	10.6	0.76	9.81	0.22	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
170		68	76	39	303.15	3.1	305.2	3.07	97.45	0.01	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
171		68	76	39	313.15	3.1	268.1	2.96	85.49	0.04	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
172		68	76	19	303.15	1.8	165.1	2.08	90.74	0.16	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
173		68	76	19	313.15	1.8	146.1	2.02	80.17	0.12	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
174		68	76	19	323.15	1.8	130	1.96	71.22	0.09	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
175		68	76	19	333.15	1.8	116.3	1.90	63.61	0.06	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
176		68	76	19	303.15	1.8	165.1	2.08	90.74	0.16	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
177		68	76	19	313.15	1.8	146.1	2.02	80.17	0.12	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
178		68	76	19	323.15	1.8	130	1.96	71.22	0.09	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
179		68	76	19	333.15	1.8	116.3	1.90	63.61	0.06	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
180		69	72	90	303.15	2.6	164.9	2.60	62.42	0.00	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
181		69	72	90	313.15	2.6	142.6	2.46	53.85	0.05	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
182		69	72	89	303.15	2.7	164.2	2.58	59.81	0.05	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
183		69	72	93	303.15	1.9	65.87	1.76	33.67	0.07	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
184		69	72	93	313.15	1.9	58.5	1.69	29.79	0.11	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
185		69	72	93	323.15	2	52.21	1.62	25.10	0.19	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
186		69	72	94	303.15	1.26	40.2	1.40	30.90	0.11	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
187		69	72	94	313.15	1.3	36.2	1.34	26.84	0.03	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
188		69	72	94	323.15	1.4	32.74	1.30	22.38	0.07	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
189		69	72	94	333.15	1.4	29.73	1.25	20.24	0.10	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
190		69	72	56	303.15	0.86	14.76	0.65	16.17	0.24	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
191		69	72	56	313.15	0.86	13.83	0.65	15.08	0.24	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
192		69	72	56	323.15	0.86	12.98	0.65	14.09	0.24	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
193		69	72	56	333.15	0.86	12.2	0.65	13.19	0.25	Gas–Liquid Chromatography	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
194		60	77	43	303.15	0.052	0.002	0.00	0.96	1.00	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
195		60	77	43	313.15	0.054	0.003	0.00	0.95	1.00	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
196		60	77	43	323.15	0.058	0.003	0.00	0.94	1.00	The Dilutor Technique	Kato, R.; Gmehling, J. (2004) Fluid Phase Equilib. 226, 37-44
197		63	80	94	298.15	1.42	33.15	1.48	22.35	0.04	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298
198		63	80	94	313.15	1.44	28.73	1.40	18.95	0.03	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298
199		63	80	94	328.15	1.45	25.13	1.33	16.33	0.09	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298
200		63	80	93	298.15	1.98	50.88	1.97	24.70	0.00	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298
201		63	80	93	313.15	2.02	43.49	1.85	20.53	0.09	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298
202		63	80	93	328.15	2.08	37.55	1.74	17.05	0.16	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
203		63	80	35	298.15	1.65	10.19	1.77	5.18	0.07	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298
204		63	80	35	313.15	1.74	9.33	1.67	4.36	0.04	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298
205		63	80	35	328.15	1.85	8.576	1.58	3.64	0.15	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298
206		63	80	27	298.15	0.386	0.762	0.04	0.97	0.90	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298
207		63	80	27	313.15	0.369	0.811	0.04	1.20	0.88	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298
208		63	80	27	328.15	0.36	0.855	0.05	1.38	0.86	Gas–Liquid Chromatography	Letcher, T. M.; Marciniak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Eng. Data 50(4), 1294-1298
209		63	81	27	298.15	0.345	0.844	0.05	1.45	0.86	Gas–Liquid Chromatography	Letcher, T. M.; Domanska, U.; Marciniak, M.; Marciniak, A. (2005) J. Chem. Thermodyn. 37(6), 587-593
210		63	81	27	303.15	0.342	0.861	0.05	1.52	0.85	Gas–Liquid Chromatography	Letcher, T. M.; Domanska, U.; Marciniak, M.; Marciniak, A. (2005) J. Chem. Thermodyn. 37(6), 587-593
211		63	81	27	308.15	0.337	0.877	0.05	1.60	0.84	Gas–Liquid Chromatography	Letcher, T. M.; Domanska, U.; Marciniak, M.; Marciniak, A. (2005) J. Chem. Thermodyn. 37(6), 587-593

Data Point	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
212	63	81	94	298.15	2.04	32.85	1.62	15.10	0.21	Gas–Liquid Chromatography	Letcher, T. M.; Domanska, U.; Marciniak, M.; Marciniak, A. (2005) J. Chem. Thermodyn. 37(6), 587-593
213	63	81	94	303.15	2.02	31.47	1.59	14.58	0.21	Gas–Liquid Chromatography	Letcher, T. M.; Domanska, U.; Marciniak, M.; Marciniak, A. (2005) J. Chem. Thermodyn. 37(6), 587-593
214	66	72	35	298.15	1.67	9.151	1.29	4.48	0.22	Gas–Liquid Chromatography	Letcher, T. M.; Marcininiak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Thermodyn. 37(12), 1327-1331
215	66	72	94	298.15	0.674	23.9	1.11	34.45	0.64	Gas–Liquid Chromatography	Letcher, T. M.; Marcininiak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Thermodyn. 37(12), 1327-1331
216	66	72	94	313.15	0.687	20.66	1.05	29.07	0.53	Gas–Liquid Chromatography	Letcher, T. M.; Marcininiak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Thermodyn. 37(12), 1327-1331
217	66	72	94	333.15	0.7	17.27	0.99	23.67	0.42	Gas–Liquid Chromatography	Letcher, T. M.; Marcininiak, A.; Marciniak, M.; Domanska, U. (2005) J. Chem. Thermodyn. 37(12), 1327-1331
218	63	74	99	313.15	1.37	36.46	1.09	25.61	0.20	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
219	63	74	99	323.15	1.47	33.34	1.06	21.68	0.28	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
220	63	74	86	313.15	1.05	82.47	1.07	77.54	0.02	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
221	63	74	86	323.15	1.13	74.17	1.05	64.64	0.07	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
222		63	74	86	333.15	1.23	66.97	1.02	53.45	0.17	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
223		63	74	22	313.15	0.51	14.59	0.42	27.61	0.18	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
224		63	74	22	323.15	0.55	14	0.42	24.46	0.23	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
225		63	74	22	333.15	0.6	13.44	0.43	21.40	0.29	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
226		63	74	32	313.15	0.79	14.63	0.81	17.52	0.02	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
227		63	74	32	323.15	0.9	13.81	0.79	14.34	0.12	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
228		63	74	32	333.15	1.04	13.05	0.78	11.55	0.25	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
229		63	74	33	313.15	1.3	21.5	0.92	15.54	0.29	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
230		63	74	55	333.15	0.74	16.6	0.34	21.43	0.54	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
231		65	70	56	363.15	1.09	14.61	0.68	12.40	0.38	Gas–Liquid Chromatography	Jork, C.; Kristen, C.; Pieraccini, D.; Stark, A.; Chiappe, C.; Beste, Y.-A.; Arlt, W. (2005) J. Chem. Thermodyn. 37(6), 537-558
232		59	70	43	363.15	0.45	0.181	0.02	0.60	0.96	Gas–Liquid Chromatography	Jork, C.; Kristen, C.; Pieraccini, D.; Stark, A.; Chiappe, C.; Beste, Y.-A.; Arlt, W. (2005) J. Chem. Thermodyn. 37(6), 537-558

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
233		59	70	27	363.15	0.4	2.739	0.17	5.85	0.58	Gas–Liquid Chromatography	Jork, C.; Kristen, C.; Pieraccini, D.; Stark, A.; Chiappe, C.; Beste, Y.-A.; Arlt, W. (2005) J. Chem. Thermodyn. 37(6), 537-558
234		63	73	43	363.15	0.1	4E-04	0.00	1.00	1.00	Gas–Liquid Chromatography	Jork, C.; Kristen, C.; Pieraccini, D.; Stark, A.; Chiappe, C.; Beste, Y.-A.; Arlt, W. (2005) J. Chem. Thermodyn. 37(6), 537-558
235		63	73	30	363.15	0.2	0.66	0.08	2.30	0.61	Gas–Liquid Chromatography	Jork, C.; Kristen, C.; Pieraccini, D.; Stark, A.; Chiappe, C.; Beste, Y.-A.; Arlt, W. (2005) J. Chem. Thermodyn. 37(6), 537-558
236		60	77	27	353.15	0.029	0.556	0.04	18.17	0.40	Static Method	Kato, R.; Gmehling, J. (2005) Fluid Phase Equilib. 231(1), 38-43
237		63	72	19	353.15	0.406	15.68	0.52	37.62	0.27	Static Method	Kato, R.; Gmehling, J. (2005) Fluid Phase Equilib. 231(1), 38-43
238		59	72	56	353.15	0.8	10.16	0.60	11.70	0.25	Static Method	Kato, R.; Gmehling, J. (2005) Fluid Phase Equilib. 231(1), 38-43
239		59	72	19	353.15	0.438	17.41	0.56	38.75	0.27	Static Method	Kato, R.; Gmehling, J. (2005) Fluid Phase Equilib. 231(1), 38-43
240		60	77	43	353.15	0.028	0.007	0.00	0.76	0.98	Static Method	Kato, R.; Gmehling, J. (2005) Fluid Phase Equilib. 231(1), 38-43
241		60	77	30	353.15	0.115	2.72	0.15	22.65	0.29	Static Method	Kato, R.; Gmehling, J. (2005) Fluid Phase Equilib. 231(1), 38-43
242		65	73	22	313.15	0.86	59.72	1.06	68.44	0.24	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
243		65	73	32	313.15	0.22	0.797	0.47	2.62	1.13	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
244		65	73	33	313.15	0.09	0.1	0.09	0.11	0.03	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
245		65	73	20	313.15	0.25	1.014	0.07	3.06	0.72	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
246		65	73	29	313.15	0.12	0.766	0.05	5.38	0.57	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
247		65	73	30	313.15	0.12	0.498	0.03	3.15	0.72	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
248		65	73	27	313.15	0.08	0.075	0.01	0.07	0.93	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
249		65	73	47	313.15	2.02	16.42	2.18	7.13	0.08	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
250		59	72	99	313.15	1.07	28.28	1.16	25.43	0.09	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
251		59	72	55	313.15	0.61	23.52	0.52	37.56	0.15	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
252		59	72	86	313.15	0.82	74.28	1.24	89.58	0.52	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
253		59	72	22	313.15	0.47	24.42	0.50	50.96	0.07	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127.
254		59	72	32	313.15	0.69	10.32	0.77	13.96	0.12	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
255		59	72	33	313.15	0.99	7.827	0.74	6.91	0.25	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
256		59	72	51	313.15	0.64	42.4	0.80	65.25	0.24	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
257		59	72	38	313.15	0.77	56.34	0.91	72.17	0.19	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
258		59	72	39	313.15	0.6	32.8	0.70	53.66	0.17	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
259		59	72	91	313.15	2.4	116.1	2.27	47.39	0.05	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
260		59	72	90	313.15	2.44	118.4	2.35	47.51	0.04	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
261		59	72	93	313.15	1.97	50.26	1.62	24.51	0.18	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
262		66	72	94	301.65	0.7785	23.08	1.10	28.64	0.41	Gas–Liquid Chromatography	Mutelet, F.; Butet, V.; Jaubert, J.-N. (2005) Ind. Eng. Chem. Res. 44, 4120 - 4127
263		66	72	94	306.95	0.776	21.91	1.08	27.24	0.39	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
264		66	72	94	312.25	0.776	20.83	1.06	25.85	0.36	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
265		66	72	94	322.75	0.777	18.92	1.02	23.35	0.32	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
266		66	72	94	322.85	0.773	18.9	1.02	23.45	0.32	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
267		66	72	94	333.25	0.777	17.25	0.99	21.20	0.28	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
268		66	72	94	343.75	0.769	15.8	0.96	19.55	0.25	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
269		66	72	33	301.75	0.67	4.878	0.64	6.28	0.05	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
270		66	72	33	301.85	0.67	4.876	0.64	6.28	0.05	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
271		66	72	33	312.25	0.68	4.72	0.64	5.94	0.06	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
272		66	72	33	312.45	0.68	4.717	0.64	5.94	0.06	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
273		66	72	33	322.85	0.69	4.566	0.63	5.62	0.08	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
274		66	72	33	323.05	0.7	4.563	0.63	5.52	0.10	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
275		66	72	33	333.45	0.71	4.417	0.63	5.22	0.11	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
276		66	72	33	343.95	0.72	4.274	0.62	4.94	0.13	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
277		66	72	107	301.75	1.11	48.21	1.02	42.43	0.08	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
278		66	72	107	312.25	1.1	43.15	0.99	38.23	0.10	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437.
279		66	72	107	322.85	1.08	38.78	0.97	34.91	0.11	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
280		66	72	107	333.35	1.06	35.06	0.94	32.07	0.11	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
281		66	72	107	343.55	1.05	31.91	0.92	29.39	0.12	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
282		66	72	107	354.05	1.03	29.09	0.90	27.24	0.12	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
283		66	72	107	364.45	1.01	26.64	0.89	25.38	0.12	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
284		66	72	107	374.95	0.99	24.47	0.87	23.71	0.12	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
285		66	72	19	301.75	0.352	20.54	0.49	57.34	0.39	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
286		66	72	19	302.25	0.352	20.46	0.49	57.11	0.39	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
287		66	72	19	312.25	0.357	18.98	0.49	52.16	0.37	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
288		66	72	19	322.85	0.362	17.58	0.49	47.57	0.34	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
289		66	72	19	333.35	0.366	16.35	0.48	43.68	0.32	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
290		66	72	19	343.85	0.371	15.25	0.48	40.11	0.30	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
291		66	72	19	354.**25**	0.375	14.27	0.48	37.06	0.28	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
292		59	71	94	301.8	2.98	68.25	2.99	21.90	0.00	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
293		59	71	94	312.3	2.94	62.68	2.85	20.32	0.03	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
294		59	71	94	323	2.88	57.63	2.72	19.01	0.05	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
295		59	71	94	333.5	2.79	53.2	2.61	18.07	0.07	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
296		59	71	94	343.9	2.69	49.26	2.50	17.31	0.07	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
297		59	71	94	354.4	2.59	45.68	2.40	16.64	0.07	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
298		65	81	27	288.15	0.405	0.732	0.04	0.81	0.90	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
299		65	81	27	298.15	0.38	0.764	0.04	1.01	0.89	Gas–Liquid Chromatography	Deenadayalu, N.; Thango, S. H.; Letcher, T. M.; Ramjugernath, D. (2006) J. Chem. Thermodyn. 38(5), 542-546
300		65	81	27	313.15	0.37	0.807	0.05	1.18	0.86	Gas–Liquid Chromatography	Deenadayalu, N.; Thango, S. H.; Letcher, T. M.; Ramjugernath, D. (2006) J. Chem. Thermodyn. 38(5), 542-546
301		66	72	110	343.55	1.11	67.3	1.34	59.63	0.21	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437.
302		66	72	110	354.05	1.07	60.17	1.30	55.23	0.22	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437.
303		66	72	110	364.45	1.02	54.1	1.27	52.04	0.24	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437.

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
304		66	72	110	374.95	0.97	48.8	1.23	49.31	0.27	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437.
305		66	72	110	385.35	0.92	44.25	1.20	47.09	0.31	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437.
306		66	72	110	395.95	0.9	40.2	1.17	43.66	0.31	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437.
307		59	71	19	323.1	1.64	95.33	1.45	57.13	0.11	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
308		59	71	19	333.6	1.63	84.91	1.41	51.09	0.14	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
309		59	71	19	343.9	1.61	76.17	1.37	46.31	0.15	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
310		59	71	19	365	1.56	61.85	1.29	38.65	0.17	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
311		59	71	19	375.4	1.54	56.17	1.25	35.48	0.19	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
312		59	71	19	386	1.5	51.12	1.22	33.08	0.18	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
313		65	81	94	288.15	1.33	27.1	1.33	19.38	0.00	Gas–Liquid Chromatography	Deenadayalu, N.; Thango, S. H.; Letcher, T. M.; Ramjugernath, D. (2006) J. Chem. Thermodyn. 38(5), 542-546
314		65	81	94	298.15	1.395	24.66	1.28	16.68	0.08	Gas–Liquid Chromatography	Deenadayalu, N.; Thango, S. H.; Letcher, T. M.; Ramjugernath, D. (2006) J. Chem. Thermodyn. 38(5), 542-546
315		65	81	94	313.15	1.36	21.58	1.21	14.86	0.11	Gas–Liquid Chromatography	Deenadayalu, N.; Thango, S. H.; Letcher, T. M.; Ramjugernath, D. (2006) J. Chem. Thermodyn. 38(5), 542-546
316		64	72	109	301.75	0.84	45.68	0.89	53.39	0.06	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
317		64	72	109	312.25	0.8	40.92	0.87	50.15	0.09	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
318		64	72	109	322.75	0.79	36.83	0.85	45.62	0.08	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
319		64	72	109	343.55	0.77	30.3	0.82	38.35	0.06	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
320		64	72	109	354.15	0.76	27.6	0.80	35.32	0.05	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
321		64	72	94	322.75	1.3	22.42	0.99	16.25	0.24	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
322		64	72	94	333.35	1.26	20.35	0.96	15.15	0.24	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
323		64	72	94	343.55	1.26	18.62	0.94	13.78	0.26	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
324		64	72	94	354.05	1.22	17.05	0.92	12.98	0.25	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
325		64	72	94	364.45	1.2	15.69	0.89	12.08	0.25	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
326		64	72	22	301.75	0.52	26.59	0.49	50.14	0.06	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
327		64	72	22	312.45	0.5	24.57	0.48	48.14	0.03	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
328		64	72	22	322.95	0.49	22.81	0.48	45.55	0.03	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
329		64	72	22	333.35	0.47	21.25	0.47	44.21	0.00	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
330		64	72	22	343.75	0.46	19.85	0.47	42.15	0.02	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
331		64	72	116	301.65	0.58	26.48	0.69	44.65	0.19	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
332		64	72	116	312.25	0.57	24.07	0.68	41.22	0.19	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
333		64	72	116	322.75	0.54	21.99	0.66	39.72	0.23	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
334		64	72	116	333.25	0.53	20.17	0.65	37.05	0.23	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
335		64	72	116	343.55	0.52	18.59	0.64	34.75	0.24	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
336		64	72	110	374.95	1.6	77.29	1.25	47.31	0.22	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
337		64	72	110	385.45	1.48	68.92	1.21	45.57	0.18	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
338		64	72	110	395.95	1.36	61.73	1.19	44.39	0.13	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
339		66	72	93	307.05	1.04	31.44	1.36	29.23	0.30	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
340		66	72	93	312.35	1.04	29.73	1.33	27.58	0.28	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
341		66	72	93	322.85	1.06	26.71	1.28	24.20	0.21	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
342		66	72	93	333.35	1.06	24.12	1.23	21.76	0.17	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
343		66	72	93	343.85	1.08	21.88	1.19	19.26	0.11	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
344		66	72	22	312.25	0.456	25.62	0.43	55.19	0.06	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
345		66	72	22	322.85	0.446	23.6	0.42	51.91	0.05	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
346		66	72	22	333.35	0.434	21.82	0.42	49.29	0.04	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
347		66	72	22	343.85	0.426	20.24	0.41	46.52	0.03	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
348		66	72	22	354.25	0.413	18.84	0.41	44.63	0.01	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
349		66	72	115	333.15	1.2	51.93	1.16	42.28	0.04	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
350		66	72	115	343.55	1.21	46.72	1.12	37.61	0.07	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
351		66	72	115	354.05	1.23	42.17	1.10	33.29	0.11	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
352		66	72	115	364.45	1.24	38.27	1.07	29.86	0.14	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
353		66	72	115	374.95	1.26	34.83	1.05	26.64	0.17	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
354		66	72	118	343.65	1.39	95.98	1.52	68.05	0.10	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
355		66	72	118	354.15	1.35	85.03	1.47	61.99	0.09	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
356		66	72	118	364.65	1.29	75.71	1.42	57.69	0.10	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
357		66	72	118	375.15	1.25	67.74	1.38	53.19	0.10	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
358		66	72	118	385.65	1.2	60.88	1.34	49.73	0.12	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
359		59	71	27	312.4	0.41	0.804	0.05	0.96	0.89	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
360		59	71	27	323	0.4	0.847	0.05	1.12	0.87	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2139
361		59	71	27	333.4	0.39	0.886	0.06	1.27	0.85	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2140
362		59	71	27	343.8	0.38	0.923	0.06	1.43	0.84	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2141
363		59	71	27	354.2	0.36	0.958	0.07	1.66	0.81	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2142
364		59	71	116	333.5	1.94	67.61	1.55	33.85	0.20	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
365		59	71	116	343.9	1.9	60.97	1.50	31.09	0.21	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2139
366		59	71	116	354.4	1.84	55.17	1.45	28.99	0.21	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2140

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
367		59	71	116	364.8	1.8	50.17	1.41	26.87	0.22	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2141
368		59	71	116	375.2	1.74	45.8	1.37	25.32	0.21	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2142
369		63	70	93	303.15	2.913	140.4	2.59	47.21	0.11	Gas–Liquid Chromatography	Zhou, Q.; Wang, L. -S. (2006) J. Chem. Eng. Data 51(5), 1698-1701
370		63	70	94	303.15	1.739	70.37	2.04	39.47	0.17	Gas–Liquid Chromatography	Zhou, Q.; Wang, L. -S. (2006) J. Chem. Eng. Data 51(5), 1698-1701
371		63	70	94	313.15	1.758	64.2	1.95	35.52	0.11	Gas–Liquid Chromatography	Zhou, Q.; Wang, L. -S. (2006) J. Chem. Eng. Data 51(5), 1698-1701
372		63	70	94	323.15	1.77	58.74	1.87	32.19	0.06	Gas–Liquid Chromatography	Zhou, Q.; Wang, L. -S. (2006) J. Chem. Eng. Data 51(5), 1698-1701
373		63	70	94	333.15	1.798	53.9	1.80	28.98	0.00	Gas–Liquid Chromatography	Zhou, Q.; Wang, L. -S. (2006) J. Chem. Eng. Data 51(5), 1698-1701
374		63	70	94	343.15	1.83	49.58	1.74	26.09	0.05	Gas–Liquid Chromatography	Zhou, Q.; Wang, L. -S. (2006) J. Chem. Eng. Data 51(5), 1698-1701
375		63	70	96	313.15	2.293	213.3	2.87	92.04	0.25	Gas–Liquid Chromatography	Zhou, Q.; Wang, L. -S. (2006) J. Chem. Eng. Data 51(5), 1698-1701
376		63	70	96	323.15	2.339	192.1	2.73	81.15	0.17	Gas–Liquid Chromatography	Zhou, Q.; Wang, L. -S. (2006) J. Chem. Eng. Data 51(5), 1698-1701

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
377		63	70	96	333.15	2.411	173.5	2.60	70.98	0.08	Gas–Liquid Chromatography	Zhou, Q.; Wang, L. -S. (2006) J. Chem. Eng. Data 51(5), 1698-1701
378		63	70	96	343.15	2.475	157.2	2.48	62.51	0.00	Gas–Liquid Chromatography	Zhou, Q.; Wang, L. -S. (2006) J. Chem. Eng. Data 51(5), 1698-1701
379		64	72	113	322.75	1.66	132.3	1.36	78.68	0.18	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
380		64	72	113	333.15	1.63	115.6	1.32	69.91	0.19	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
381		64	72	113	364.55	1.44	79.55	1.21	54.25	0.16	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
382		64	72	113	374.95	1.33	71.01	1.18	52.39	0.11	Gas–Liquid Chromatography	Heintz, A.; Vasiltsova, T. V.; Safarov, J.; Bich, E.; Verevkin, S. P. (2006) J. Chem. Eng. Data 51(2), 648-655
383		66	72	119	322.75	0.868	56.74	1.12	64.37	0.29	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
384		66	72	119	333.25	0.874	50.79	1.09	57.12	0.25	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
385		66	72	119	343.65	0.877	45.74	1.06	51.15	0.21	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
386		66	72	119	354.15	0.884	41.33	1.03	45.76	0.17	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
387		66	72	113	322.75	1.04	86.29	1.37	81.97	0.32	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
388		66	72	113	333.25	1.03	76.36	1.33	73.14	0.29	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
389		66	72	113	343.65	1.01	68.02	1.29	66.34	0.27	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
390		66	72	113	354.15	0.99	60.82	1.25	60.43	0.26	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
391		66	72	114	354.15	1.6	120	1.71	74.00	0.07	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
392		66	72	114	364.65	1.52	105.8	1.65	68.64	0.09	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
393		66	72	114	375.15	1.44	93.85	1.59	64.17	0.11	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
394		66	72	114	385.65	1.38	83.62	1.54	59.59	0.12	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
395		66	72	112	322.75	0.681	36.57	0.82	52.71	0.20	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
396		66	72	112	333.25	0.683	33.25	0.80	47.68	0.18	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
397		66	72	112	343.65	0.685	30.38	0.79	43.34	0.15	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
398		66	72	112	354.15	0.688	27.83	0.78	39.45	0.13	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
399		66	72	109	301.75	0.578	31.41	0.80	53.34	0.39	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
400		66	72	109	312.25	0.576	28.43	0.79	48.36	0.37	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
401		66	72	109	322.85	0.574	25.83	0.77	43.99	0.34	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
402		66	72	109	333.35	0.572	23.58	0.76	40.23	0.32	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
403		66	72	116	301.75	0.453	19.77	0.60	42.65	0.34	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
404		66	72	116	312.25	0.45	18.11	0.60	39.23	0.32	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
405		66	72	116	322.85	0.444	16.63	0.59	36.46	0.32	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
406		66	72	116	333.35	0.439	15.35	0.58	33.96	0.32	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
407		66	72	92	322.85	1.55	37.16	1.53	22.97	0.01	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
408		66	72	92	333.35	1.55	33.24	1.47	20.45	0.05	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437

Data Point	ILs	Cation	Anion	Solutes	T /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)	Experimental method	Reference
409		66	72	92	343.85	1.54	29.89	1.42	18.41	0.08	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
410		66	72	92	354.25	1.53	27.02	1.37	16.66	0.10	Gas–Liquid Chromatography	Heintz, A.; Verevkin, S. P.; Ondo, D. (2006) J. Chem. Eng. Data 51(2), 434-437
411		59	71	22	312.2	0.81	49.29	1.00	59.85	0.23	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
412		59	71	22	333.4	0.8	41.23	0.95	50.54	0.19	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
413		59	71	22	343.9	0.78	37.94	0.93	47.64	0.19	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
414		59	71	22	354.3	0.77	35.05	0.91	44.52	0.18	Gas–Liquid Chromatography	Sumartschenkowa, I. A.; Verevkin, S. P.; Vasiltasova, T. V.; Bich, E.; Heintz, A.; Shevelyova, M. P.; Kabo, G. J. (2006) J. Chem. Eng. Data 51(6), 2138
							ARD =	#34.3075	0.2099			

C. Data for Validation of Modified Model

Table C.1: Validation of modified COSMO-SAC model for ILs

Data Point	ILs	Cation	Anion	Solutes	*T* /K	γ^{∞}	COSMO-SAC 2002	This Work	RD COSMO-SAC 2002	RD (This Work)
1		699	850	18	318.15	0.94	90.657042	0.933685	95.443661	0.00671804
2		699	850	18	323.15	0.95	85.120639	0.9241643	88.600672	0.027195522
3		699	850	18	323.15	0.95	85.120639	0.9241643	88.600672	0.027195522
4		699	850	18	333.15	0.97	75.362159	0.9062118	76.692947	0.065761032
5		699	850	18	343.15	0.98	67.082161	0.8895817	67.451184	0.09226353
6		699	850	32	333.15	0.56	8.1010878	0.6272324	13.466228	0.120057798
7		699	850	32	343.15	0.57	7.7444852	0.6196988	12.586816	0.087190822
8		699	850	89	353.15	1.72	82.963088	1.331959	47.234353	0.225605235
9		699	850	92	353.15	1.73	52.548155	1.1857635	29.374656	0.314587601
10		59	845	19	318.15	2.46	123.7797	2.2784492	49.316952	0.073801144
11		59	845	19	323.15	2.47	117.58039	2.2362361	46.603398	0.094641253
12		59	845	19	333.15	2.47	106.42521	2.1567105	42.087128	0.126837854
13		59	845	19	343.15	2.48	96.702927	2.0831337	37.993116	0.160026746
14		59	845	19	353.15	2.49	88.188206	2.0148878	34.41695	0.190808099
15		59	845	32	318.15	0.7	1.8957114	0.9621975	1.7081592	0.374567901
16		59	845	32	323.15	0.73	1.9658491	0.9650972	1.692944	0.322050993
17		59	845	32	333.15	0.78	2.1028011	0.9696031	1.6958989	0.243080843
18		59	845	32	343.15	0.83	2.2346847	0.9725577	1.6923912	0.171756297
19		59	845	32	353.15	0.89	2.3608613	0.9741523	1.6526531	0.094553161
20		59	845	39	318.15	4.48	173.43818	3.2239699	37.713879	0.280363851
21		59	845	39	323.15	4.46	165.27943	3.1538496	36.058169	0.292858835
22		59	845	39	333.15	4.48	150.45707	3.0223531	32.584167	0.325367604
23		59	845	39	343.15	4.41	137.38365	2.9014124	30.152756	0.34208335
24		59	845	39	353.15	4.38	125.80931	2.7898699	27.723586	0.363043412
25		59	845	94	318.15	4.51	42.788473	4.0202729	8.4874663	0.108586939
26		59	845	94	323.15	4.5	41.892093	3.9295667	8.309354	0.126762953
27		59	845	94	333.15	4.48	40.157472	3.7594122	7.9637215	0.160845482
28		59	845	94	343.15	4.48	38.499794	3.6028528	7.5937041	0.195791781
29		59	845	94	353.15	4.46	36.917624	3.4584036	7.2774942	0.224573181
							ARD =		**32.4888**	**0.1807**

Table C.2: Effect of Cation size on IDAC

γ^{∞}	**COSMO-SAC 2002**	**This Work**	**RD COSMO-SAC 2002**	**RD (This Work)**
1.35	39.18	1.4	28.02222222	0.037037037
1.2	31.61	1.28	25.34166667	0.066666667
0.89	24.53	1.14	26.56179775	0.280898876
0.68	20.65	1.04	29.36764706	0.529411765

Table C.3: Effect of Anion Size on IDAC

Solutes	***T* /K**	γ^{∞}	**COSMO-SAC 2002**	**This Work**	**RD COSMO-SAC 2002**	**RD (This Work)**
Benzene	323.15	2.8	57.56	2.71	19.55	0.029
Benzene	333.15	2.83	53.34	2.6	17.84	0.07
Benzene	323.15	1.21	28.71	1.24	22.73	0.02
Benzene	333.15	1.18	26.18	1.2	21.02	0.01
Benzene	323.15	4.5	41.89	3.9	8.3	0.13
Benzene	333.15	4.48	40.15	3.73	7.9600	0.1600

Table C.4: Comparison of Henry's law constant of CO_2 in IL using COSMO-SAC 2010 and This Work

Data Point	ILs Cation	Anion	Solutes	*T* /K	This Work	Pi	Hi_exp	Hi_COSMO-SAC 2010	Hi_This Work	RD COSMO-SAC 2010	RD This Work	Reference
1	63	70	CO_2	283.1	0.7986	4.506	4.08	3.59	3.5987	0.120098	0.117966	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
2	63	70	CO_2	298.1	0.768	6.4405	5.65	5.2	4.9463	0.079646	0.124549	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
3	63	70	CO_2	303.38	0.7581	7.2547	6.16	5.87	5.4998	0.047078	0.107175	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
4	63	72	CO_2	283.15	0.4801	4.5116	2.53	2.14	2.1662	0.15415	0.143794	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
5	63	72	CO_2	298.1	0.4655	6.4405	3.3	3	2.9984	0.090909	0.091394	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
6	63	72	CO_2	303	0.4611	7.1935	3.347	3.33	3.3172	0.005079	0.008903	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

Data Point	ILs Cation	Anion	Solutes	*T* /K	This Work	Pi	Hi_exp	Hi_COSMO-SAC 2010	Hi_This Work	RD COSMO-SAC 2010	RD This Work	Reference
7	65	72	CO_2	298.1	0.3848	6.4405	3	2.27	2.4785	0.243333	0.173833	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
8	65	72	CO_2	303.03	0.3814	7.1984	3.3	2.53	2.7456	0.233333	0.168	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
9	65	70	CO_2	303	0.5569	7.1935	5.39	3.87	4.0064	0.282004	0.256698	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
10	59	72	CO_2	283.1	0.54	4.506	2.53	2.67	2.4333	0.055336	0.038221	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
11	59	72	CO_2	298.1	0.5227	6.4405	3.56	3.72	3.3665	0.044944	0.054354	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
12	59	72	CO_2	303.45	0.517	7.266	4.01	4.16	3.7567	0.037406	0.063167	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

Data Point	ILs	Cation	Anion	Solutes	*T* /K	This Work	Pi	Hi_exp	Hi_COSMO-SAC 2010	Hi_This Work	RD COSMO-SAC 2010	RD This Work	Reference
13		63	74	CO_2	283.1	0.5679	4.5 06	3.88	3.8	2.5588	0.020619	0.340515	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
14		63	74	CO_2	293.17	0.5569	5.7 459	4.68	4.82	3.1996	0.029915	0.316325	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
15		63	74	CO_2	298.1	0.5518	6.4 405	5.34	5.39	3.554	0.009363	0.334457	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
16		63	74	CO_2	303	0.547	7.1 935	5.98	6	3.935	0.003344	0.341973	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
17		59	70	CO_2	298	0.9549	6.4 258	8.1	6.36	6.1359	0.214815	0.242481	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
									ARD =		**0.0983**	**0.1720**	

```
A = 140.54;
B = -4735;
C = -21.268;
D = 0.040909;
E = 1;

Pi = (exp(A + (B/TEMP) + C*log(TEMP) + D*(TEMP^E)))/1000000;


fugacity = Pi;
Hi = fugacity*IDAC(JJ);
```

Where:

A, B, C, D, and E are constants.

Pi is partial pressure of CO_2

IDAC(JJ) is the IDAC of solute (CO_2 in this case), designated by JJ in the Matlab programme

Hi is the henry's law constant

Table C.5: Henry's law constant for CO_2 in BMIM-TF2N

Data Point ILs	Cation	Anion	Solutes	*T* /K	IDAC (This Work)	Pi	Hi_exp	Hi_This Work	Reference
1	63	72	CO_2	280	0.4835	4.17	1.88	2.016	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
2	63	72	CO_2	300	0.4638	6.72	2.71	3.119	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
3	63	72	CO_2	320	0.4471	10.4	3.72	4.631	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
4	63	72	CO_2	340	0.4327	15.4	5.05	6.682	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
5	63	72	CO_2	300	0.4638	6.72	2.8	3.119	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
6	63	72	CO_2	350	0.4263	18.7	7.3	7.964	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
7	63	72	CO_2	400	0.3997	45.8	1.21	18.3	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
8	63	72	CO_2	450	0.3802	108	1.71	40.97	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
9	63	72	CO_2	500	0.3653	254	2.24	92.73	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
10	63	72	CO_2	313	0.4525	8.97	3.7	4.06	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

Data Point ILs	Cation	Anion	Solutes	*T* /K	IDAC (This Work)	Pi	Hi_exp	Hi_This Work	Reference
11	63	72	CO_2	283	0.4801	4.51	2.53	2.16601916	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
12	63	72	CO_2	298	0.4655	6.45	3.3	3.00149745	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
13	63	72	CO_2	323	0.4447	11.1	4.87	4.9148244	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
14	63	72	CO_2	283	0.4799	4.54	2.39	2.17644248	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
15	63	72	CO_2	293	0.4701	5.76	3	2.70622467	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
16	63	72	CO_2	303	0.461	7.23	3.64	3.3317853	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
17	63	72	CO_2	303	0.4609	7.23	3.66	3.33253745	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
18	63	72	CO_2	303	0.4609	7.24	3.65	3.33474977	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
19	63	72	CO_2	313	0.4524	9.01	4.35	4.07730024	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
20	63	72	CO_2	313	0.4523	9.02	4.32	4.07897709	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

Data Point	ILs	Cation	Anion	Solutes	*T* /K	IDAC (This Work)	Pi	Hi_exp	Hi_This Work	Reference
21		63	72	CO_2	323	0.4446	11.1	5.08	4.92074388	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
22		63	72	CO_2	323	0.4444	11.1	5.11	4.94470548	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
23		63	72	CO_2	324	0.4443	11.2	5.02	4.95674409	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
24		63	72	CO_2	334	0.437	13.7	5.91	5.9677594	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
25		63	72	CO_2	334	0.437	13.7	5.77	5.9748388	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
26		63	72	CO_2	344	0.4302	16.6	6.65	7.14329892	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
27		63	72	CO_2	344	0.4302	16.6	6.7	7.14467556	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
28		63	72	CO_2	303	0.4611	7.19	3.34	3.31692285	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
29		63	72	CO_2	313	0.4527	8.94	4.12	4.04885826	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
30		63	72	CO_2	323	0.4448	11	4.77	4.90089536	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

Data Point ILs	Cation	Anion	Solutes	*T* /K	IDAC (This Work)	Pi	Hi_exp	Hi_This Work	Reference
31	63	72	CO_2	298	0.4655	6.45	3.3	3.00149745	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
32	63	72	CO_2	333	0.4374	13.5	4.87	5.9088366	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
33	63	72	CO_2	294	0.4694	5.86	2.05	2.75002684	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
34	63	72	CO_2	298	0.4656	6.43	2.25	2.99185248	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
35	63	72	CO_2	303	0.4611	7.19	2.53	3.31692285	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
36	63	72	CO_2	313	0.4527	8.94	3.14	4.04885826	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
37	63	72	CO_2	323	0.4448	11	3.84	4.90089536	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
38	63	72	CO_2	333	0.4375	13.5	4.62	5.8926875	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
39	63	72	CO_2	343	0.4307	16.4	5.47	7.04569209	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
40	63	72	CO_2	348	0.4275	18	5.93	7.69102425	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

Data Point ILs	Cation	Anion	Solutes	*T* /K	IDAC (This Work)	Pi	Hi_exp	Hi_This Work	Reference
41	63	72	CO_2	353	0.4244	19.8	6.41	8.38669572	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
42	63	72	CO_2	363	0.4185	23.8	7.42	9.94569435	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
43	63	72	CO_2	298	0.4655	6.45	3.7	3.00149745	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
44	63	72	CO_2	313	0.4525	8.97	4.1	4.060011	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
45	63	72	CO_2	283	0.4801	4.51	2.8	2.16601916	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
46	63	72	CO_2	293	0.4702	5.74	3.07	2.70049966	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
47	63	72	CO_2	298	0.4655	6.45	3.43	3.00149745	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
48	63	72	CO_2	303	0.461	7.22	4.2	3.3273136	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
49	63	72	CO_2	313	0.4525	8.97	4.5	4.060011	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
50	63	72	CO_2	323	0.4447	11.1	5.1	4.9148244	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

Table C6: Henry's law constant for CO_2 in EMIM-TF2N

Data Point	ILs Cation	Anion	Solutes	*T* /K	IDAC (This Work)	Pi	Hi_exp	Hi_This Work	Reference
1	59	72	CO_2	298.15	0.5227	6.4479	3.9	3.37	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
2	59	72	CO_2	313.15	0.5073	8.9724	5	4.5519	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
3	59	72	CO_2	328.15	0.4937	12.2297	6.3	6.0375	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
4	59	72	CO_2	343.15	0.4814	16.4058	7.8	7.8985	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
5	59	72	CO_2	300	0.5207	6.7249	3.4	3.5014	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
6	59	72	CO_2	350	0.4763	18.6817	8.7	8.8978	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
7	59	72	CO_2	400	0.4449	45.7926	14	20.3753	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

Data Point	ILs	Cation	Anion	Solutes	*T* /K	IDAC (This Work)	Pi	Hi_exp	Hi_This Work	Reference
8		59	72	CO_2	450	0.4219	107.7528	20.7	45.4574	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
9		59	72	CO_2	500	0.4043	253.8401	26.2	102.6266	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
10		59	72	CO_2	303.45	0.517	7.266	3.96	3.7567	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
11		59	72	CO_2	303.45	0.517	7.266	3.95	3.7567	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
12		59	72	CO_2	298.15	0.5227	6.4479	3.59	3.37	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
13		59	72	CO_2	313.15	0.5073	8.9724	4.76	4.5519	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
14		59	72	CO_2	323.15	0.4981	11.052	5.71	5.5045	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
15		59	72	CO_2	303	0.5175	7.1935	3.9	3.7226	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

Data Point ILs	Cation	Anion	Solutes	*T* /K	IDAC (This Work)	Pi	Hi_exp	Hi_This Work	Reference
16	59	72	CO_2	303.63	0.5168	7.2951	3.81	3.7704	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
17	59	72	CO_2	303.87	0.5166	7.3341	3.86	3.7888	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
18	59	72	CO_2	313.87	0.5066	9.1107	4.59	4.6158	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
19	59	72	CO_2	313.92	0.5066	9.1204	4.62	4.6203	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
20	59	72	CO_2	313.95	0.5066	9.1262	4.54	4.6229	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
21	59	72	CO_2	323.96	0.4973	11.2362	5.42	5.5881	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
22	59	72	CO_2	323.98	0.4973	11.2408	5.46	5.5902	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
23	59	72	CO_2	324.05	0.4973	11.2568	5.39	5.5975	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

Data Point	ILs	Cation	Anion	Solutes	*T* /K	IDAC (This Work)	Pi	Hi_exp	Hi_This Work	Reference
24		59	72	CO_2	324.12	0.4972	11.2729	5.45	5.6048	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
25		59	72	CO_2	334.07	0.4887	13.7561	6.29	6.7225	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
26		59	72	CO_2	334.1	0.4887	13.7642	6.34	6.7261	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
27		59	72	CO_2	334.16	0.4886	13.7804	6.39	6.7333	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
28		59	72	CO_2	343.99	0.4808	16.6714	7.25	8.0156	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
29		59	72	CO_2	344.23	0.4806	16.7479	7.29	8.0493	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
30		59	72	CO_2	283.43	0.5396	4.5431	2.49	2.4515	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
31		59	72	CO_2	293.39	0.5279	5.7757	3.11	3.049	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
32		59	72	CO_2	303.39	0.5171	7.2563	3.79	3.7522	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
33		59	72	CO_2	323.22	0.498	11.0678	5.38	5.5117	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

Data Point	ILs	Cation	Anion	Solutes	*T* /K	IDAC (This Work)	Pi	Hi_exp	Hi_This Work	Reference
34		59	72	CO_2	343.07	0.4815	16.3807	7.3	7.8874	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
35		59	72	CO_2	313.15	0.5073	8.9724	4.66	4.5519	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
36		59	72	CO_2	323.15	0.4981	11.052	5.5	5.5045	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
37		59	72	CO_2	333.15	0.4895	13.509	6.4	6.612	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
38		59	72	CO_2	298.15	0.5227	6.4479	3.9	3.37	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
39		59	72	CO_2	313.15	0.5073	8.9724	4.8	4.5519	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.
40		59	72	CO_2	298.15	0.5227	6.4479	3.56	3.37	Lee, B.-S., Lin, S.-T., Screening of ionic liquids for CO_2 capture using the COSMO-SAC model. Chem. Eng. Sci. (2014). http://dx.doi.org/10.1016/j.ces.2014.08.017.

D. Computer Codes and Files

D.1 COSMO-SAC VT-2002 Sigma Averaging Fortran Programme (https://apps.che.vt.edu/Liu-2013/VT-Databases.html. Accessed on 05/07/2023)

```
PROGRAMME SIGMAPROFILEV2
!**************************************************************************
**************
!CREATED USING DIGITAL VISUAL FORTRAN 6.0 (2006)
!
!       This programme reads the modified COSMO output file (in text format)
from Accelrys'
! Materials Studio DMol3 and averages the surface segment charge densities
per
! Klamt (1995), Klamt et al (1998), Klamt et al (2000), Lin and Sandler
(2002) to
! establish the segment charges for the "sigma-profile".  This programme
creates
! a text file that MS Excel can read and plot.
!
!       THIS PROGRAMME WRITTEN BY:
!               RICHARD OLDLAND (roldland@vt.edu)               MIKE ZWOLAK
(zwolak@caltech.edu)
!               DEPARTMENT OF CHEMICAL ENGINEERING              PHYSICS
DEPARTMENT
!               VIRGINIA TECH                                   CALIFORNIA
INSTITUTE OF TECHNOLOGY
!               BLACKSBURG, VA 24060                            PASADENA, CA
91125
!
!       EDITED MARCH 2006 BY:
!               ERIC MULLINS (pmullins@vt.edu)
!               DEPARTMENT OF CHEMICAL ENGINEERING
!               VIRGINIA TECH
!               BLACKSBURG, VA 24060
!
!
!       VALUES READ FROM THE DATA FILE:
!       ATOM = ATOM NUMBER IN MOLECULE
!       POSXAU = X-CORDINATE OF THE SEGMENT POSITION IN ATOMIC UNITS
!       POSYAU = Y-CORDINATE OF THE SEGMENT POSITION IN ATOMIC UNITS
!       POSZAU = Z-CORDINATE OF THE SEGMENT POSITION IN ATOMIC UNITS
!       POSXA = X-CORDINATE OF THE SEGMENT POSITION IN ANGSTROMS
!       POSYA = Y-CORDINATE OF THE SEGMENT POSITION IN ANGSTROMS
!       POSZA = Z-CORDINATE OF THE SEGMENT POSITION IN ANGSTROMS
!       A = SURFACE SEGMENT AREA; APPROXIMATED AS CIRCULAR (ANGSTROMS SQUARED)
!       CHG = CHARGE OF THE SURFACE SEGMENT (SIGMA, e)
!       SIGMA = RATIO OF SURFACE CHARGE TO AREA (SIGMA/A, e/A**2)
!       POTENT = SURFACE POTENTIAL
!
!       FROM SEGMENT CHARGE AVERAGING:
!       REFF = RADIUS OF THE AREA THAT AFFECTS THE SURFACE SEGMENT CHARGE
(ANGSTROMS)
!        DMN = DISTANCE BETWEEN CALCULATED SEGEMENT AND SEGEMENTS AFFECTING IT
(ANGSTROMS)
!       RAD = RADIUS OF THE PARTICULAR SURFACE SEGMENT (ASSUMED CIRCULAR,
ANGSTROMS SQUARED)
```

```
!       SIGMANEW = NEW AVERAGED SIGMA VALUE
!       SIGMASUM = SUMMATION OF EFFECTS FROM OTHER SURFACE SEGMENTS
!       NORMDIST = NORMALIZATION FACTOR
!       NORMSUM = SUMMATION OF ALL NORMALIZATION FACTORS
!
!       REQUIRED INPUT (ON PROMPT):
!               NAME OF FILE (INCLUDING LOCATION AND EXTENSION)
!               NAME OF CHEMICAL (THIS WILL APPEAR IN THE OUTPUT FILE)
!               NUMSEGMENT = THE NUMBER OF SURFACE SEGMENTS
!
!  THE OUTPUT FILE "'CHEMICAL'SIGMA-PROFILE.TXT" IS THE SORTED SIGMA PROFILE
!
!  LITERATURE CITED:
!  Klamt, A. Conductor-like Screening Model for Real Solvents: A New Approach
to the
!       Quantitative Calculation of Solvation Phenomena. J. Phys. Chem 1995,
99, 2224.
!  Klamt, A.; Jonas, V.; Burger, T.; Lohrenz, J. Refinement and
Parameterization of
!       COSMO-RS. J. Phys. Chem A 1998, 102, 5074.
!  Klamt, A.; Eckert, F.; COSMO-RS: A Novel and Efficient Method for the a
Priori
!       Prediction of Thermophysical Data of Liquids.  Fluid Phase Equilibria
2000,
!       172, 43.
!  Lin, S.T.; Sandler, S. A Priori Phase Equilibrium Prediction from a
Segment
!       Contribution Solvation Model. Ind. Eng. Chem. Res, 2002, 41, 899
!  Lin, S.T.;  Quantum Mechanical Approaches to the Prediction of Phase
Equilibria:
!       Solvation Thermodynamics and Group Contribution Methods, PhD.
Dissertation,
!       University of Delaware, Newark, DE, 2000
!**********************************************************************
**************
IMPLICIT NONE

CHARACTER(128):: FILEINDEX, FILEOUTPUT
CHARACTER(16):: CHEMICAL
CHARACTER(1) :: RESPONSE
CHARACTER (256) :: FILENAME
INTEGER :: I, J, K, F, M, N, O, DUMBI, TMP, NUMSEGMENT
INTEGER, DIMENSION (:), ALLOCATABLE :: ATOM
INTEGER, DIMENSION (1500) :: FILEIN, FILEOUT
REAL*8 :: REFF, PI
REAL*8, DIMENSION (:), ALLOCATABLE :: POSXAU, POSYAU, POSZAU, POSXA, POSYA,
POSZA, A
REAL*8, DIMENSION (:), ALLOCATABLE :: CHG, SIGMA, POTENT, SIGMANEW, SIGMASUM,
RAD, NORMDIST
REAL*8, DIMENSION (:), ALLOCATABLE :: NORMSUM, DMN
REAL*8, DIMENSION(1:51) :: CHGDEN,SP

! ESTABLISH INPUT FILE UNIT NUMBERS
DO N = 1, 1500
   FILEIN(N) = N+20
END DO

! ESTABLISH OUTPUT FILE UNIT NUMBERS
DO O = 1, 1500
```

```
   FILEOUT(O) = O+1521
END DO

!ESTABLISH CONSTANTS
PI = 3.14159265358979
REFF = 0.81764200000000

!REPETITION LOOP TO CALCULATE MULTIPLE P(S)
DO F = 1, 1500

   ! INPUT VARIABLES DEFINED FROM ARRAYS FILENAME AND NUMBSEGMENT
   !FILELOOP = 'C:\COSMO\VT-2006_AMBER\'//FILENAME(F)
   !FILEOUTPUT = 'C:\PROFILES\VT-2006_AMBER\'//FILENAME(F)
   !NUMSEGMENT = NUMBSEGMENT(F)

   !ESTABLISHING THE COSMO FILE TO READ
   WRITE(*,*) "TYPE THE NAME OF THE FILE YOU WISH TO READ IN,"
   WRITE(*,*) "INCLUDING LOCATION (MAX 256 CHARACTERS), AND HIT ENTER"
   READ (*,*) FILENAME

   !ESTABLISH THE CHEMICAL NAME
   WRITE(*,*) "TYPE IN THE NAME OF THE CHEMICAL (MAX 16 CHARACTERS), AND HIT
ENTER"
   WRITE(*,*) "SIGMA PROFILE OUTPUT FILE WILL BE CREATED IN C:\PROFILES\"
   WRITE(*,*) "IF THIS DIRECTORY DOES NOT EXIST, PLEASE CREATE IT AT THIS
TIME."
   READ (*,*) CHEMICAL

   FILEOUTPUT = 'C:\PROFILES\'//CHEMICAL//'.TXT'

   !OPEN THE COSMO FILE WITH ALL SEGMENTS AND CORRESPONDING CHARGE DENSITIES
   OPEN(UNIT=FILEIN(F), FILE = FILENAME, STATUS = "OLD", ACTION = "READ",
POSITION = "REWIND")

   !ESTABLISH THE NUMBER OF SURFACE SEGMENTS AND ALLOCATE THE ARRAYS
   WRITE(*,*) "TYPE THE NUMBER OF SURFACE SEGMENTS, FROM THE COSMO OUTPUT,
AND HIT ENTER"
   READ (*,*) NUMSEGMENT

   ALLOCATE(ATOM(NUMSEGMENT), POSXAU(NUMSEGMENT), POSYAU(NUMSEGMENT), &
        POSZAU(NUMSEGMENT), POSXA(NUMSEGMENT), POSYA(NUMSEGMENT), &
                 POSZA(NUMSEGMENT), A(NUMSEGMENT), CHG(NUMSEGMENT),
SIGMA(NUMSEGMENT), &
                 POTENT(NUMSEGMENT), SIGMANEW(NUMSEGMENT),
SIGMASUM(NUMSEGMENT), &
                 RAD(NUMSEGMENT), NORMDIST(NUMSEGMENT), NORMSUM(NUMSEGMENT),
DMN(NUMSEGMENT))

   !READ THE COSMO FILE AND ESTABLISH THE DATA ARRAYS
   DO I = 1, NUMSEGMENT
      READ(FILEIN(F),*)
DUMBI,ATOM(I),POSXAU(I),POSYAU(I),POSZAU(I),CHG(I),A(I),SIGMA(I),POTENT(I)
         !CONVERT THE POSITIONS FROM ATOMIC UNITS TO ANGSTROMS AND ASSIGN NEW
ARRAYS
         POSXA(I) = POSXAU(I) * 0.529177249
         POSYA(I) = POSYAU(I) * 0.529177249
         POSZA(I) = POSZAU(I) * 0.529177249
         RAD(I) = SQRT(A(I)/PI)
```

```
   END DO

   !CLOSE COSMO FILE
   CLOSE(FILEIN(F))


   !BEGIN AVERAGING SURFACE CHARGES
   DO J=1, NUMSEGMENT
          SIGMANEW(J) = 0.D0
          NORMSUM(J)=0.D0

          DO K=1, NUMSEGMENT
                 DMN(K) = SQRT((POSXA(K)-POSXA(J))**2+(POSYA(K)-POSYA(J))**2+
&
                              (POSZA(K)-POSZA(J))**2)
                 SIGMASUM(K)=
SIGMA(K)*(RAD(K)**2*REFF**2)/(RAD(K)**2+REFF**2)* &
                                    DEXP(-(DMN(K)**2)/(RAD(K)**2+REFF**2))
                 NORMDIST(K) =(RAD(K)**2*REFF**2)/(RAD(K)**2+REFF**2)* &
                                    DEXP(-(DMN(K)**2)/(RAD(K)**2+REFF**2))
                 NORMSUM(J) = NORMSUM(J) + NORMDIST(K)
                 SIGMANEW(J) = SIGMANEW(J) + SIGMASUM(K)
      END DO

        SIGMANEW(J) = SIGMANEW(J)/NORMSUM(J)
   END DO

   !CONTAINS AVERAGED SIGMA-PROFILE
   OPEN (FILEOUT(F), FILE = FILEOUTPUT)

   !SETTING CHGDEN MATRIX
   DO J=1,51
          SP(J)=0.D0
          CHGDEN(J) = -0.025D0+0.001D0*DBLE(J-1)
   END DO

   !SIGMA PROFILE SORTING TAKEN FROM LIN DISSERTATION**
   DO J=1,NUMSEGMENT
          TMP=INT((SIGMANEW(J)-CHGDEN(1))/0.001D0)
          SP(TMP+1)=SP(TMP+1)+A(J)*(CHGDEN(TMP+2)-SIGMANEW(J))/0.001D0
          SP(TMP+2)=SP(TMP+2)+A(J)*(SIGMANEW(J)-CHGDEN(TMP+1))/0.001D0
   END DO

   DO J=1,51
          WRITE(FILEOUT(F),*) CHGDEN(J),SP(J)
   END DO

   CLOSE(FILEOUT(F))

     DEALLOCATE(ATOM, POSXAU, POSYAU, POSZAU, &
        POSXA, POSYA, POSZA, A, &
            CHG, SIGMA, POTENT, SIGMANEW, &
            SIGMASUM, RAD, NORMDIST, NORMSUM, &
            DMN)

   !REPEAT SIGMA PROFILE CALCULATION FOR ANOTHER COMPOUND
   WRITE (*,*) "DO YOU WISH TO CALCULATE ANOTHER SIGMA PROFILE (Y or N)"
   READ (*,*) RESPONSE
```

```
   IF (RESPONSE=="N") EXIT

END DO

END PROGRAMME SIGMAPROFILEV2
```

D.2 COSMO-SAC VT-2002 Activity Coefficient Fortran Programme

(https://apps.che.vt.edu/Liu-2013/VT-Databases.html. Accessed on 05/07/2023)

```
PROGRAMME GAMMA1
!************************************************************************
*******
!       This programme uses the sigma profiles of two pure components to
calculate
!   the liquid-phase activity coefficients in a solution.  This is the first
!   step in predicting VLE for mixtures.
!
!       This programme uses the COSMO-SAC model as published (Lin, S.T.,
!       S.I. Sandler, Ind. Eng. Chem. Res. 41, (2002), 899-913).
!
!       THIS PROGRAMME WRITTEN BY:
!         RICHARD OLDLAND (roldland@vt.edu)    MIKE ZWOLAK
(zwolak@caltech.edu)
!         DEPARTMENT OF CHEMICAL ENGINEERING   PHYSICS DEPARTMENT
!         VIRGINIA TECH                        CALIFORNIA INSTITUTE OF
TECHNOLOGY
!         BLACKSBURG, VA 24060                 PASADENA, CA 91125
!
!       PHYSICAL CONSTANTS AND PARAMETERS:
!         EO = PERMITTIVITY IN A VACUUM (e**2*mol/Kcal*Angstrom)
!         AEFFPRIME = EFFECTIVE SURFACE AREA (ANGSTROMS**2) --FROM LIN
!         RGAS = IDEAL GAS CONSTANT (Kcal/mol*K)
!         VNORM = VOLUME NORMALIZATION CONSTANT (A**3) --FROM LIN
!         ANORM = AREA NORMALIZATION CONSTANT (A**2) --FROM LIN
!         COORD = THE COORIDINATION NUMBER --FROM LIN
!         CHB = HYDROGEN BONDING COEFFICIENT (Kcal/mole*Angstroms**4/e**2)
!         SIGMAHB = CUTOFF VALUE FOR HYDROGEN BONDING (e/Angstrom**2)
!         EPS = RELATIVE PERMITTIVITY --FROM LIN
!         ALPHAPRIME = A CONSTANT USED IN THE MISFIT ENERGY CALCULATION
!
!       INPUT PARAMETERS:
!         SYSTEMP = THE SYSTEM TEMPERATURE (K)
!         COMP = NUMBER OF COMPONENTS IN THE SYSTEM --SET TO 2 FOR BINARY
!         SYSCOMP = NAMES OF COMPONENTS IN THE SYSTEM
!         VCOSMO = CAVITY VOLUME FROM COSMO OUTPUT (A**3)
!         ACOSMO = MOLECULAR SURFACE AREA FROM COSMO OUTPUT (A**2) --THE SUM
!              OF THE INDIVIDUAL PROFILE.
!
!
!       LITERATURE CITED:
!  Klamt, A. Conductor-like Screening Model for Real Solvents: A New Approach
to the
!       Quantitative Calculation of Solvation Phenomena. J. Phys. Chem 1995,
99, 2224.
!  Klamt, A.; Jonas, V.; Burger, T.; Lohrenz, J. Refinement and
Parameterization of
!       COSMO-RS. J. Phys. Chem A 1998, 102, 5074.
!  Klamt, A.; Eckert, F.; COSMO-RS: A Novel and Efficient Method for the a
Priori
!       Prediction of Thermophysical Data of Liquids.  Fluid Phase Equilibria
2000,
!       172, 43.
!  Lin, S.T.; Sandler, S. A Priori Phase Equilibrium Prediction from a
Segment
```

```
!       Contribution Solvation Model. Ind. Eng. Chem. Res, 2002, 41, 899
!  Lin, S.T.;  Quantum Mechanical Approaches to the Prediction of Phase
Equilibria:
!       Solvation Thermodynamics and Group Contribution Methods, PhD.
Dissertation,
!       University of Delaware, Newark, DE, 2000
!
!
!       PROGRAMME CURRENTLY SETUP FOR BINARY MIXTURES ONLY
!**********************************************************************
******
IMPLICIT NONE
REAL,PARAMETER:: EO = 2.395*10.0**-4, AEFFPRIME = 7.5, RGAS = 0.001987
REAL,PARAMETER:: VNORM = 66.69, ANORM = 79.53
REAL :: FPOL, ALPHA, ALPHAPRIME, COORD, EPS, SYSTEMP, SIGMAHB, CHB, FRAC1,
FRAC2
REAL :: SYSPRES, SIGMAACC, SIGMADON, SUMMATION, BOTTHETA, BOTPHI, PHI1, PHI2
REAL :: THETA1, THETA2, L1, L2, GAMMASG1, GAMMASG2, GAMMA, GAMMA2, SUMGAMMA1
REAL :: SUMGAMMA2, N1, N2, LNGAMMA, LNGAMMA2
INTEGER :: I, J, K, L, M, COMPSEG, COUNT, COMP
REAL, DIMENSION(2):: VCOSMO, ACOSMO, RNORM, QNORM
REAL, DIMENSION(:), ALLOCATABLE:: COUNTER, DENOM, PROFILE, NUMER, SEGGAMMA
REAL, DIMENSION(:), ALLOCATABLE:: SEGGAMMAOLD, CONVERG
REAL, DIMENSION(:,:), ALLOCATABLE:: SIGMA, DELTAW, SEGGAMMAPR, SEGGAMMAOLDPR,
CONPR
CHARACTER (16), DIMENSION(2):: SYSCOMP
CHARACTER (256), DIMENSION(2):: FILENAME
CHARACTER :: ANSWER
CHARACTER (256):: OUTPUT

COMPSEG = 51 !NUMBER OF INTERVALS FOR THE SIGMA PROFILE
EPS = 3.667 !(LIN AND SANDLER USE A CONSTANT FPOL WHICH YEILDS EPS=3.68)
COORD = 10.0 !(KLAMT USED 7.2)
SIGMAHB = 0.0084
CHB = 85580.0
COMP =2

FPOL = (EPS-1.0)/(EPS+0.5)
ALPHA = (0.3*AEFFPRIME**(1.5))/(EO)
ALPHAPRIME = FPOL*ALPHA


ALLOCATE(SIGMA(COMPSEG,COMP), COUNTER(COMPSEG), PROFILE(COMPSEG),
NUMER(COMPSEG),&
        DENOM(COMPSEG), DELTAW(COMPSEG,COMPSEG), SEGGAMMA(COMPSEG),
SEGGAMMAOLD(COMPSEG), &
        CONVERG(COMPSEG), SEGGAMMAPR(COMPSEG,COMP),
SEGGAMMAOLDPR(COMPSEG,COMP), &
        CONPR(COMPSEG,COMP))


!DEFINE SYSTEM TEMPERATURE (K)
WRITE(*,*) "ENTER IN THE SYSTEM TEMPERATURE (K)"
READ(*,*) SYSTEMP

!DEFINE THE SYSTEM AS WELL AS THE AREA AND VOL FROM THE COSMO CALCULATION
DO I=1, COMP
        WRITE(*,*) "ENTER THE NAME OF COMPONENT", I
        READ(*,*) SYSCOMP(I)
```

```
        WRITE(*,*) "ENTER THE LOCATION AND NAME OF THE  ", SYSCOMP(I), "SIGMA
PROFILE (256 character max)"
        READ(*,*) FILENAME(I)
        WRITE(*,*) "ENTER THE CAVITY VOLUME FOR COMPONENT",I
        READ(*,*) VCOSMO(I)
END DO

!OPEN THE SIGMA PROFILES FOR THE PURE COMPONENTS
OPEN(UNIT=1, FILE=FILENAME(1), STATUS="OLD", ACTION="READ",
POSITION="REWIND")
OPEN(UNIT=2, FILE=FILENAME(2), STATUS="OLD", ACTION="READ",
POSITION="REWIND")

!READ INDIVIDUAL SIGMA PROFILES; COUNTER IS THE SIGMA VALUE, SIGMA IS
P(SIGMA)
DO K = 1, COMP
        ACOSMO(K) =0.0
        DO J=1, COMPSEG
                READ(K,*)COUNTER(J), SIGMA(J,K)
                ACOSMO(K)=ACOSMO(K)+SIGMA(J,K)
        END DO
END DO
CLOSE(1)
CLOSE(2)

!ESTABLISH OUTPUT FILES.  THE PROGRAMME CREATES A FILE FOR THE GAMMA-X DATA
WRITE(*,*) "ENTER THE LOCATION AND NAME FOR THE OUTPUT FILE, INCLUDE
EXTENSION."
READ (*,*) OUTPUT
OPEN(UNIT=11, FILE = OUTPUT, STATUS="NEW")
WRITE(11,*) "SYSTEMP", SYSTEMP, "KELVIN"
5  FORMAT (1X,A10,5X,A12,5X,A12,5X,A12,5X,A12)
6  FORMAT (1X,A10,5X,A9,5X,A10,7X,A10,5X,A10)
WRITE(11,6) "MOLE FRAC", "GAMMA1", "GAMMA2", "LNGAMMA1", "LNGAMMA2"
WRITE(11,5) "X1", SYSCOMP(1), SYSCOMP(2), SYSCOMP(1), SYSCOMP(2)



!VARYING MOLE FRACTIONS // ONLY WORKS FOR BINARY MIXTURE
DO FRAC1 = 0.005, 0.995, 0.01
FRAC2 = 1.0 - FRAC1
!CALCULATE THE MIXTURE SIGMA PROFILE
        DO J =1,COMPSEG
                NUMER(J) = FRAC1*SIGMA(J,1) + FRAC2*SIGMA(J,2)
                DENOM(J) = FRAC1*ACOSMO(1) + FRAC2*ACOSMO(2)
                PROFILE(J) = NUMER(J)/DENOM(J)

        END DO
        DO I = 1, COMPSEG
                DO K = 1, COMPSEG
                        IF (COUNTER(I)>=COUNTER(K)) THEN
                                SIGMAACC = COUNTER(I)
                                SIGMADON = COUNTER(K)
                        END IF
                        IF (COUNTER(I)<COUNTER(K)) THEN
                                SIGMADON = COUNTER(I)
                                SIGMAACC = COUNTER(K)
                        END IF
```

```
                DELTAW(I,K) = (ALPHAPRIME/2.0)*(COUNTER(I)+COUNTER(K))**2.0 +
CHB *   &
                        MAX(0.0,(SIGMAACC - SIGMAHB))*MIN(0.0,(SIGMADON +
SIGMAHB))
                END DO
        END DO


!ITERATION FOR SEGMENT ACTIVITY COEF. (MIXTURE)
SEGGAMMA = 1.0
DO
        SEGGAMMAOLD = SEGGAMMA
        DO I = 1, COMPSEG
                SUMMATION = 0.0
                DO K = 1, COMPSEG
                        SUMMATION = SUMMATION + PROFILE(K)* SEGGAMMAOLD(K) * &
                                EXP(-DELTAW(I,K)/(RGAS*SYSTEMP))
                END DO
                SEGGAMMA(I)=EXP(-LOG(SUMMATION))
                SEGGAMMA(I)=(SEGGAMMA(I)+SEGGAMMAOLD(I))/2.0
        END DO
        DO I=1, COMPSEG
                CONVERG(I)=ABS((SEGGAMMA(I)-SEGGAMMAOLD(I))/SEGGAMMAOLD(I))
        END DO
IF (MAXVAL(CONVERG) <=0.000001) EXIT
END DO

!ITERATION FOR SEGMENT ACITIVITY COEF (PURE SPECIES)
DO L = 1, COMP
        SEGGAMMAPR (:,L) = 1.0
        DO
                SEGGAMMAOLDPR (:,L) = SEGGAMMAPR (:,L)
                DO I = 1, COMPSEG
                        SUMMATION = 0.0
                        DO K = 1, COMPSEG
                                SUMMATION = SUMMATION +
(SIGMA(K,L)/ACOSMO(L))*SEGGAMMAOLDPR(K,L) * &
                                        EXP(-DELTAW(I,K)/(RGAS*SYSTEMP))
                        END DO
                        SEGGAMMAPR(I,L)=EXP(-LOG(SUMMATION))

        SEGGAMMAPR(I,L)=(SEGGAMMAPR(I,L)+SEGGAMMAOLDPR(I,L))/2.0
                END DO
                DO I=1, COMPSEG
                        CONPR(I,L)=ABS((SEGGAMMAPR(I,L)-
SEGGAMMAOLDPR(I,L))/SEGGAMMAOLDPR(I,L))
                END DO

        IF (MAXVAL(CONPR) <=0.000001) EXIT
        END DO
END DO

!THE STAVERMAN-GUGGENHEIM EQUATION
DO I = 1,COMP
        RNORM(I) = VCOSMO(I)/VNORM
        QNORM(I) = ACOSMO(I)/ANORM
END DO

BOTTHETA = FRAC1*QNORM(1) + FRAC2*QNORM(2)
```

```
BOTPHI = FRAC1*RNORM(1) + FRAC2*RNORM(2)

THETA1 = (FRAC1*QNORM(1))/BOTTHETA
THETA2 = (FRAC2*QNORM(2))/BOTTHETA

PHI1 = (FRAC1*RNORM(1))/BOTPHI
PHI2 = (FRAC2*RNORM(2))/BOTPHI

L1 = (COORD/2.0)*(RNORM(1)-QNORM(1))-(RNORM(1)-1.0)
L2 = (COORD/2.0)*(RNORM(2)-QNORM(2))-(RNORM(2)-1.0)

!GAMMASG1 AND GAMMASG2 ARE ACTUALLY LNGAMMASG
GAMMASG1 = LOG(PHI1/FRAC1)+(COORD/2)*QNORM(1)*LOG(THETA1/PHI1)+L1-
(PHI1/FRAC1)* &
        (FRAC1*L1 + FRAC2*L2)
GAMMASG2 = LOG(PHI2/FRAC2)+(COORD/2)*QNORM(2)*LOG(THETA2/PHI2)+L2-
(PHI2/FRAC2)* &
        (FRAC1*L1 + FRAC2*L2)


!CALCULATION OF GAMMAS
SUMGAMMA1 = 0.0
SUMGAMMA2 = 0.0
DO I = 1, COMPSEG
        SUMGAMMA1 = SUMGAMMA1
+((SIGMA(I,1)/AEFFPRIME)*(LOG(SEGGAMMA(I)/(SEGGAMMAPR(I,1)))))
        SUMGAMMA2 = SUMGAMMA2
+((SIGMA(I,2)/AEFFPRIME)*(LOG(SEGGAMMA(I)/(SEGGAMMAPR(I,2)))))
END DO


GAMMA =EXP(SUMGAMMA1 + (GAMMASG1))
GAMMA2=EXP(SUMGAMMA2 + (GAMMASG2))
LNGAMMA = LOG(GAMMA)
LNGAMMA2 = LOG(GAMMA2)


WRITE(11,*) FRAC1,GAMMA, GAMMA2, LNGAMMA, LNGAMMA2


END DO


END PROGRAMME GAMMA1
```

D.3 COSMO-SAC Sigma Averaging Matlab Programme

```
%       PROGRAMME SIGMAPROFILE
%
!*************************************************************************
******
% % !  This programme reads the modified COSMO output file (in text format) from
Accelrys'
% ! Materials Studio DMol3 and averages the surface segment charge densities per
% ! Klamt (1995), Klamt et al (1998), Klamt et al (2000), Lin and Sandler (2002) to
% ! establish the segment charges for the "sigma-profile".
% !
% !    THIS PROGRAMME WRITTEN BY:
% !          RICHARD OLDLAND (roldland@vt.edu)              MIKE ZWOLAK
(zwolak@caltech.edu)
% !          DEPARTMENT OF CHEMICAL ENGINEERING             PHYSICS DEPARTMENT
% !          VIRGINIA TECH                                  CALIFORNIA INSTITUTE OF
TECHNOLOGY
% !          BLACKSBURG, VA 24060                           PASADENA, CA 91125
% !
% !    EDITED MARCH 2006 BY:
% !          ERIC MULLINS (pmullins@vt.edu)
% !          DEPARTMENT OF CHEMICAL ENGINEERING
% !          VIRGINIA TECH
% !          BLACKSBURG, VA 24060
% !
% ! TRANSLATED TO MATLAB BY
% !     SAIDU M. WAZIRI (smwaziri@kfum.edu.sa)
% !     DEPARTMENT OF CHEMICAL ENGINEERING
% !     KING FAHD UNIVERSITY OF PETROLEUM & MINERALS
% !     DHAHRAN 31261
% !     SAUDI ARABIA
% !
% !    VALUES READ FROM THE DATA FILE:
% !    ATOM = ATOM NUMBER IN MOLECULE
% !    POSXAU = X-CORDINATE OF THE SEGMENT POSITION IN ATOMIC UNITS
% !    POSYAU = Y-CORDINATE OF THE SEGMENT POSITION IN ATOMIC UNITS
% !    POSZAU = Z-CORDINATE OF THE SEGMENT POSITION IN ATOMIC UNITS
% !    POSXA = X-CORDINATE OF THE SEGMENT POSITION IN ANGSTROMS
% !    POSYA = Y-CORDINATE OF THE SEGMENT POSITION IN ANGSTROMS
% !    POSZA = Z-CORDINATE OF THE SEGMENT POSITION IN ANGSTROMS
% !    A = SURFACE SEGMENT AREA; APPROXIMATED AS CIRCULAR (ANGSTROMS SQUARED)
% !    CHG = CHARGE OF THE SURFACE SEGMENT (SIGMA, e)
% !    SIGMA = RATIO OF SURFACE CHARGE TO AREA (SIGMA/A, e/A**2)
% !    POTENT = SURFACE POTENTIAL
% !
% !    FROM SEGMENT CHARGE AVERAGING:
% !    REFF = RADIUS OF THE AREA THAT AFFECTS THE SURFACE SEGMENT CHARGE (ANGSTROMS)
% !       DMN = DISTANCE BETWEEN CALCULATED SEGEMENT AND SEGEMENTS AFFECTING IT
(ANGSTROMS)
% !    RAD = RADIUS OF THE PARTICULAR SURFACE SEGMENT (ASSUMED CIRCULAR, ANGSTROMS
SQUARED)
% !    SIGMANEW = NEW AVERAGED SIGMA VALUE
% !    SIGMASUM = SUMMATION OF EFFECTS FROM OTHER SURFACE SEGMENTS
% !    NORMDIST = NORMALIZATION FACTOR
% !    NORMSUM = SUMMATION OF ALL NORMALIZATION FACTORS
% !
```

```
% !    REQUIRED INPUT (ON PROMPT):
% !          NAME OF FILE (INCLUDING LOCATION AND EXTENSION)
% !          NAME OF CHEMICAL (THIS WILL APPEAR IN THE OUTPUT FILE)
% !          NUMSEGMENT = THE NUMBER OF SURFACE SEGMENTS
% !
% !  THE OUTPUT FILE "'CHEMICAL'SIGMA-PROFILE.TXT" IS THE SORTED SIGMA PROFILE
% !
% !  LITERATURE CITED:
% !  Klamt, A. Conductor-like Screening Model for Real Solvents: A New Approach to
the
% !       Quantitative Calculation of Solvation Phenomena. J. Phys. Chem 1995, 99,
2224.
% !  Klamt, A.; Jonas, V.; Burger, T.; Lohrenz, J. Refinement and Parameterization of
% !    COSMO-RS. J. Phys. Chem A 1998, 102, 5074.
% !  Klamt, A.; Eckert, F.; COSMO-RS: A Novel and Efficient Method for the a Priori
% !    Prediction of Thermophysical Data of Liquids.  Fluid Phase Equilibria 2000,
% !    172, 43.
% !  Lin, S.T.; Sandler, S. A Priori Phase Equilibrium Prediction from a Segment
% !       Contribution Solvation Model. Ind. Eng. Chem. Res, 2002, 41, 899
% !  Lin, S.T.;  Quantum Mechanical Approaches to the Prediction of Phase Equilibria:
% !    Solvation Thermodynamics and Group Contribution Methods, PhD. Dissertation,
% !    University of Delaware, Newark, DE, 2000
%
!*************************************************************************
******


%  clear all
%  clc


function sig = Sigma_Average(data,opt2)
format long G
%     !ESTABLISH CONSTANTS
PI = 3.14159265358979;
REFF = 0.81764200000000;

%COSMO FILE WITH ALL SEGMENTS AND CORRESPONDING CHARGE DENSITIES
NUMSEGMENT = length(data);

%         !READ THE COSMO FILE AND ESTABLISH THE DATA ARRAYS
DUMBI  = data(:,1);
ATOM   = data(:,2);
POSXAU = data(:,3);
POSYAU = data(:,4);
POSZAU = data(:,5);
CHG    = data(:,6);


opt1 = opt2;

switch opt1

    % When calculating using COSMO files from VT_2005 Database
    case 1
        A      = data(:,7);
        SIGMA  = data(:,8);
```

```
        POTENT = data(:,9);

        % When calculating using COSMO files from DMOL V_2017
    case 2
        A      = data(:,7)*(0.529177249^2);
        SIGMA  = data(:,8)*(1/0.529177249^2);
        POTENT = data(:,9)*0.5302;

        case 3
        A      = data(:,7);
        SIGMA  = data(:,8);
        POTENT = data(:,9);
end


%!CONVERT THE POSITIONS FROM ATOMIC UNITS TO ANGSTROMS AND ASSIGN NEW ARRAYS
POSXA = POSXAU * 0.529177249 ;
POSYA = POSYAU * 0.529177249 ;
POSZA = POSZAU * 0.529177249 ;
RAD = sqrt(A./PI) ;

DMN = zeros (1,NUMSEGMENT);
SIGMASUM = zeros (1,NUMSEGMENT);
NORMDIST = zeros (1,NUMSEGMENT);
NORMSUM = zeros (1,NUMSEGMENT);
SIGMANEW = zeros (1,NUMSEGMENT);


%         !BEGIN AVERAGING SURFACE CHARGES
for J=1:NUMSEGMENT
    SIGMANEW(J) = 0.0;
    NORMSUM(J)=0.0;

    for K=1:NUMSEGMENT
        DMN(K) = sqrt((POSXA(K)-POSXA(J))^2+(POSYA(K)-POSYA(J)) ...
            ^2+ (POSZA(K)-POSZA(J))^2);
        SIGMASUM(K)= SIGMA(K)*(RAD(K)^2*REFF^2)/(RAD(K)^2+ ...
            REFF^2)* exp(-(DMN(K)^2)/(RAD(K)^2+REFF^2));
        NORMDIST(K) =(RAD(K)^2*REFF^2)/(RAD(K)^2+REFF^2)* ...
            exp(-(DMN(K)^2)/(RAD(K)^2+REFF^2));
        NORMSUM(J) = NORMSUM(J) + NORMDIST(K);
        SIGMANEW(J) = SIGMANEW(J) + SIGMASUM(K);
    end

    SIGMANEW(J) = SIGMANEW(J)/NORMSUM(J);
end

% !SETTING CHGDEN MATRIX
for J=1:51
    SP(J)=0.00;
    CHGDEN(J) = -0.025 + 0.001*double(J-1);
end

% !SIGMA PROFILE SORTING TAKEN FROM LIN DISSERTATION**
for J=1:NUMSEGMENT
    TMP=fix((SIGMANEW(J)-CHGDEN(1))/0.0010);
    SP(TMP+1)=SP(TMP+1)+A(J)*(CHGDEN(TMP+2)-SIGMANEW(J))/0.0010;
```

```
    SP(TMP+2)=SP(TMP+2)+A(J)*(SIGMANEW(J)-CHGDEN(TMP+1))/0.0010;

end
sig = [ CHGDEN' SP'];
disp ( [ CHGDEN' SP'] );
figure
plot( CHGDEN,SP)
xlabel (['Screening Charge Density, \sigma (e/A^2)'])
ylabel(['Sigma Profile, P(\sigma)* A, (A^2) '])
```

D.4 Main Optimization File

```
% clear all; clc; close all;

% Data
DataFile;

format shortg

rng default % for reproducibility

opt = input('Select \n 1 = Genetic Algorithm \n 2 = Particle Swarm \n 3 = Simulated
Annealing \n 4 = LSQCURVEFIT \n 5 = PATTERNSEARCH \n 6 = LSQNONLIN \n 7 = FMINCON \n
8 = FMINUNC \n 9 = FMINSEARCH \n>> ');

OF_OPTION = input('Select \n 1 = LEAST SQUARE \n 2 = ABSOLUTE ERROR \n 3 = ABSOLUTE
RELATIVE ERROR \n >> ');

tic

switch opt
    case 1
        % GENETIC ALGORITHM
        MaxGen = 5 + 100*NVARS;
        options = optimoptions(@ga,'Display','iter','MaxGenerations',
MaxGen,'MutationFcn',@mutationadaptfeasible,'PlotFcn',...
            {@gaplotbestf,@gaplotbestindiv,@gaplotexpectation,@gaplotstopping},
'PopulationSize', 1000);
        A = []; b =[];  Aeq = []; beq =[];
        NONLCON = [];
        [par,fval, exitflag, output, population, scores] = ga(@(par) Obj_Fcn(par,
XDATA, YDATA),NVARS,A,b,Aeq,beq,lb,ub,NONLCON); %,options);

    case 2
        % PARTICLE SWARM OPTIMISATION
        %         Swarm_Size = 50+100*NVARS;
        Swarm_Size = 3;
        %         options = optimoptions('particleswarm','SwarmSize',100,'Display',
'iter','HybridFcn',@fmincon);
        options = optimoptions(@particleswarm,'SwarmSize',Swarm_Size, 'Display',
'iter');
%         options.FunValCheck = 'on';
options.MaxIter = 10;
        [par,fval, exitflag, output] = particleswarm(@(par)Obj_Fcn(par, XDATA, YDATA,
OF_OPTION),NVARS, lb, ub, options);

    case 3
        % SIMULATED ANNEALING
                options = saoptimset;
                options.Display = 'iter';
                options.MaxFunEvals = 100;
%         options = optimoptions(@simulannealbnd,'Display', 'iter');
        par = simulannealbnd(@(par) Obj_Fcn(par, XDATA,
YDATA,OF_OPTION),par0,lb,ub,options);

    case 4
        % LSQCURVEFIT
```

```
        options = optimoptions(@lsqcurvefit,'Display', 'iter','Algorithm','levenberg-
marquardt');
        options.TolX = 1.0000e-20;
        options.TolFun = 1.0000e-20;
        options.MaxFunEvals = 1000;
        %         par0 = [7.5 85580 0.0084 66.69 79.53];
        [par,resnorm,res,exitflag,output, lambda,jac] =
lsqcurvefit(@COSMO_SAC_TERNARY, par0, XDATA, YDATA,lb,ub,options);
%         [par,resnorm,res,exitflag,output] = lsqcurvefit(@COSMO_SAC_2007_TERNARY,
par0, XDATA, YDATA,lb,ub,options);
%         [par,resnorm,res,exitflag,output] = lsqcurvefit(@COSMO_SAC_TERNARY_META,
par0, XDATA, YDATA,lb,ub,options);
        % [par,resnorm,res,exitflag,output] = lsqcurvefit(@COSMO_SAC_TERNARY_META,
par0, XDATA, YDATA,lb,ub,options);
        % [par,resnorm,res,exitflag,output] = lsqcurvefit(@COSMO_SAC_TERNARY_NEW,
par0, XDATA, YDATA,lb,ub,options);

    case 5
        % PATTERN SEARCH
        options = optimoptions(@patternsearch);%,'Display',
'iter','Algorithm','levenberg-marquardt');
        options.Display = 'iter';
        A = []; b =[];  Aeq = []; beq =[];
        [par,fval,exitflag] = patternsearch(@(par) Obj_Fcn(par, XDATA,
YDATA),par0,A,b,Aeq,beq,lb,ub,options);

    case 6
        % LSQNONLIN
        options = optimoptions(@lsqnonlin);%,'Display',
'iter','Algorithm','levenberg-marquardt');
        options.Display = 'iter';
        [par,resnorm, residual, exitflag] = lsqnonlin(@(par) Obj_Fcn(par, XDATA,
YDATA, OF_OPTION),par0,lb,ub,options);

    case 7
        %         % FMINCON
        options = optimoptions(@fmincon,'Display', 'iter');
%                 options = optimoptions(@fmincon,'UseParallel', true,'Display',
'iter','Algorithm','interior-point');
        %         options.Display = 'iter';
        A = []; b =[];  Aeq = []; beq =[];
%                 options.TolX = 1.0000e-20;
%                 options.TolFun = 1.0000e-20;
%                 options.MaxFunEvals = 1;
        [par,fval,exitflag,output,lambda] = fmincon(@(par) Obj_Fcn(par, XDATA, YDATA,
OF_OPTION),par0,A,b,Aeq,beq,lb,ub,[],options);

        % FMINCON
        %         opts = optimoptions(@fmincon,'levenberg-marquardt');
        %         options.Display = 'iter';
        % %       A = []; b =[];  Aeq = []; beq =[];
        %         options.TolX = 1.0000e-20;
        %         options.TolFun = 1.0000e-20;
        %         options.MaxFunEvals = 100000;
        %         problem =
createOptimProblem('lsqnonlin','objective',@Obj_Fcn,'x0',@par0,'lb',[0 0 0],'ub',[inf
inf inf],'nonlcon',@circularConstraint,'options',opts);
```

```
        %         gs = GlobalSearch;
        %         [par,fval,exitflag,output,lambda] = run(gs,problem);
    case 8
        % FMINUNC
        options = optimoptions(@fminunc);%,'Display', 'iter','Algorithm','levenberg-
marquardt');
        options.Display = 'iter';
        options.TolX = 1.0000e-20;
        options.TolFun = 1.0000e-20;
        options.MaxFunEvals = 100000;
        [par,fval,exitflag,output,lambda] = fminunc(@(par) Obj_Fcn(par, XDATA,
YDATA,OF_OPTION),par0,options);

    case 9
        % FMINSEARCH
        options = optimset(@fminsearch);%,'Display', 'iter','Algorithm','levenberg-
marquardt');
        options.Display = 'iter';
        [par,fval,exitflag,output] = fminsearch(@(par) Obj_Fcn(par, XDATA, YDATA,
OF_OPTION),par0,options);

    case 10
        % NLM
        nlm = fitnlm(XDATA,YDATA,@COSMO_SAC_TERNARY,par0);
        disp(nlm)
        par = nlm.Coefficients.Estimate
        ci = coefCI(nlm,0.5)
        numCoefficients = nlm.NumCoefficients
        mse = nlm.MSE
        res = nlm.Residuals
        r2 = nlm.Rsquared
        ssr = nlm.SSR
        sst = nlm.SST
        sse = nlm.SSE
        rmse = nlm.RMSE
        [p,F,r] = coefTest(nlm)
        dof = nlm.DFE
        cov = nlm.CoefficientCovariance
        coeff_names = nlm.CoefficientNames
        leverage= nlm.Diagnostics.Leverage
        cooksDistance =nlm.Diagnostics.CooksDistance
        hatMatrix = nlm.Diagnostics.HatMatrix
        formula = nlm.Formula
        fitted = nlm.Fitted
        iterative = nlm.Iterative
        logLikelihood = nlm.LogLikelihood
        modelCriterion = nlm.ModelCriterion
end
toc

% Plot Results
YMODEL_orig = COSMO_SAC_TERNARY(par0,XDATA);
YMODEL = COSMO_SAC_TERNARY(par,XDATA);
figure(1)
% plot(XDATA(:,1),YDATA,'o', XDATA(:,1),YMODEL,'-')
plot(XDATA(:,1),YDATA,'o', XDATA(:,1),YMODEL,'+')
title('Plot of Temperature VS IDAC for Pred and Exp')
```

```
xlabel('Temperature'), ylabel('IDAC')
% hold on

figure(2)
plot(YMODEL,YDATA,'o', YDATA,YDATA,'-')
% plot(YDATA,YMODEL_orig,'*',YDATA,YMODEL,'o',YDATA,GammaRS,'+', YDATA,YDATA,'-')
% plot(YDATA,YMODEL_orig,'o', YDATA,YDATA, '-')
title('Plots of Exp IDAC VS Orig Pred IDAC and Optim Pred IDAC')
xlabel('Experimental IDAC'), ylabel('Predicted IDAC')
disp(par);

[res, r2, r2adj, SSE, RMSE] = stat_data(par,YMODEL,YDATA)

% [std,varresid,r2,cor,vcv,varinf]=regdata(par,YMODEL,YDATA,jac)

fileID = fopen('testdata.txt','w');
fprintf(fileID,'%6s\r\n','par');
fprintf(fileID,'%12.4f',par);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','r2');
fprintf(fileID,'%12.4f',r2);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','r2adj');
fprintf(fileID,'%12.4f',r2adj);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','res');
fprintf(fileID,'%12.4f',res);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','RMSE');
fprintf(fileID,'%12.4f',RMSE);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','SSE');
fprintf(fileID,'%12.4f',SSE);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','exitflag');
fprintf(fileID,'%12.0f',exitflag);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fclose(fileID);
```

D.5 Modified COSMO-SAC for Optimization Matlab Programme

```
function IDAC = COSMO_SAC_TERNARY(PAR,INPUT_DATA)
% PROGRAMME GAMMA1
%
!*************************************************************************
% !    This programme uses the sigma profiles of two pure components to calculate
% !   the liquid-phase activity coefficients in a solution.  This is the first
% !   step in predicting VLE for mixtures.
% !
% !    This programme uses the COSMO-SAC model as published (Lin, S.T.,
% !    S.I. Sandler, Ind. Eng. Chem. Res. 41, (2002), 899-913).
% !
% !    THIS PROGRAMME WRITTEN BY:
% !      RICHARD OLDLAND (roldland@vt.edu)     MIKE ZWOLAK (zwolak@caltech.edu)
% !      Eric Mullins (pmullins@vt.edu)     PHYSICS DEPARTMENT
% !      DEPARTMENT OF CHEMICAL ENGINEERING    CALIFORNIA INSTITUTE OF TECHNOLOGY
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% !      BLACKSBURG, VA 24060
% !
% ! TRANSLATED TO MATLAB BY
% !     SAIDU M. WAZIRI (smwaziri@kfum.edu.sa)
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% !     DHAHRAN 31261
% !     SAUDI ARABIA
% !
% !
% !    PHYSICAL CONSTANTS AND PARAMETERS:
% !      EO = PERMITTIVITY IN A VACUUM (e**2*mol/Kcal*Angstrom)
% !      AEFFPRIME = EFFECTIVE SURFACE AREA (ANGSTROMS**2) --FROM LIN
% !      RGAS = IDEAL GAS CONSTANT (Kcal/mol*K)
% !      VNORM = VOLUME NORMALIZATION CONSTANT (A**3) --FROM LIN
% !      ANORM = AREA NORMALIZATION CONSTANT (A**2) --FROM LIN
% !      COORD = THE COORIDINATION NUMBER --FROM LIN
% !      CHB = HYDROGEN BONDING COEFFICIENT (Kcal/mole*Angstroms**4/e**2)
% !      SIGMAHB = CUTOFF VALUE FOR HYDROGEN BONDING (e/Angstrom**2)
% !      EPS = RELATIVE PERMITTIVITY --FROM LIN
% !      ALPHAPRIME = A CONSTANT USED IN THE MISFIT ENERGY CALCULATION
% !
% !    INPUT PARAMETERS:
% !      SYSTEMP = THE SYSTEM TEMPERATURE (K)
% !      COMP = NUMBER OF COMPONENTS IN THE SYSTEM --SET TO 2 FOR BINARY
% !      SYSCOMP = NAMES OF COMPONENTS IN THE SYSTEM
% !      VCOSMO = CAVITY VOLUME FROM COSMO OUTPUT (A**3)
% !      ACOSMO = MOLECULAR SURFACE AREA FROM COSMO OUTPUT (A**2) --THE SUM
% !           OF THE INDIVIDUAL PROFILE.
% !
% !
% !    LITERATURE CITED:
% !  Klamt, A. Conductor-like Screening Model for Real Solvents: A New Approach to
the
% !       Quantitative Calculation of Solvation Phenomena. J. Phys. Chem 1995, 99,
2224.
% !  Klamt, A.; Jonas, V.; Burger, T.; Lohrenz, J. Refinement and Parameterization of
% !    COSMO-RS. J. Phys. Chem A 1998, 102, 5074.
% !  Klamt, A.; Eckert, F.; COSMO-RS: A Novel and Efficient Method for the a Priori
```

```
% !    Prediction of Thermophysical Data of Liquids.  Fluid Phase Equilibria 2000,
% !    172, 43.
% !  Lin, S.T.; Sandler, S. A Priori Phase Equilibrium Prediction from a Segment
% !       Contribution Solvation Model. Ind. Eng. Chem. Res, 2002, 41, 899
% !  Lin, S.T.;  Quantum Mechanical Approaches to the Prediction of Phase Equilibria:
% !    Solvation Thermodynamics and Group Contribution Methods, PhD. Dissertation,
% !    University of Delaware, Newark, DE, 2000
% !
% !
% !    PROGRAMME CURRENTLY SETUP FOR BINARY MIXTURES ONLY
% !*************************************************************************
% IMPLICIT NONE
% REAL,PARAMETER:: EO = 2.395*10.0**-4, AEFFPRIME = 7.5, RGAS = 0.001987
% REAL,PARAMETER:: VNORM = 66.69, ANORM = 79.53
% REAL :: FPOL, ALPHA, ALPHAPRIME, COORD, EPS, SYSTEMP, SIGMAHB, CHB, FRAC1, FRAC2
% REAL :: SYSPRES, SIGMAACC, SIGMADON, SUMMATION, BOTTHETA, BOTPHI, PHI1, PHI2
% REAL :: THETA1, THETA2, L1, L2, GAMMASG1, GAMMASG2, GAMMA, GAMMA2, SUMGAMMA1
% REAL :: SUMGAMMA2, N1, N2, LNGAMMA, LNGAMMA2
% INTEGER :: I, J, K, L, M, COMPSEG, COUNT, COMP
% REAL, DIMENSION(2):: VCOSMO, ACOSMO, RNORM, QNORM
% REAL, DIMENSION(:), ALLOCATABLE:: COUNTER, DENOM, PROFILE, NUMER, SEGGAMMA
% REAL, DIMENSION(:), ALLOCATABLE:: SEGGAMMAOLD, CONVERG
% REAL, DIMENSION(:,:), ALLOCATABLE:: SIGMA, DELTAW, SEGGAMMAPR, SEGGAMMAOLDPR, CONPR
% CHARACTER (16), DIMENSION(2):: SYSCOMP
% CHARACTER (256), DIMENSION(2):: FILENAME
% CHARACTER :: ANSWER
% CHARACTER (256):: OUTPUT

DataFile

TEMP_INPUT = INPUT_DATA(:,1);
ID1_INPUT = INPUT_DATA(:,2);
ID2_INPUT = INPUT_DATA(:,3);
ID3_INPUT = INPUT_DATA(:,4);

numDATA = length(TEMP_INPUT);

IDAC = zeros(numDATA,1);

for JJ = 1:numDATA
    TEMP = TEMP_INPUT(JJ);
    ID1 = ID1_INPUT(JJ);
    ID2 = ID2_INPUT(JJ);
    ID3 = ID3_INPUT(JJ);
  sigma = ones(51,2);
% Scale = [1 1e-4 1e3 1e-1 1e-1];

% PARAMETERS
EO = 2.395e-4;
% AEFFPRIME = 7.5; % Optimize for species that do not have the capacity for hydrogen
bonding
AEFFPRIME = PAR(1);
%  AEFFPRIME = PAR(1)*Scale(1);
% m = PAR(2);
m = 0.5;
% m = 1.0;
% m = PAR(5);
```

```
Cne = PAR(6);
% A = PAR(2);
% B = PAR(3);
% C = PAR(7);
% Cne = 0;
% Ces = 9254;
% Ces = PAR(2);
% D = 1.0;
% D = PAR(2);
% C1 = 1;
% C2 = 1;
% m = PAR(3);
C1 = PAR(4);
C2 = PAR(5);
% LTS = PAR(4);
% LTS = 1720;
RGAS = 0.001987;
% VNORM = 66.69; % No need to optimize the volume normalization constant
VNORM = PAR(3);
% ANORM = 79.53; % No need to optimize the area normalization constant
ANORM = PAR(2);
COMPSEG = 51;  %NUMBER OF INTERVALS FOR THE SIGMA PROFILE FROM LIN & SANDLER SIGMA
AVERAGEING PROGRAME
% COMPSEG = 26;  %NUMBER OF INTERVALS FOR THE SIGMA PROFILE FROM LIN & SANDLER SIGMA
AVERAGEING PROGRAME
% COMPSEG = 11;  %NUMBER OF INTERVALS FOR THE SIGMA PROFILE FROM LIN & SANDLER SIGMA
AVERAGEING PROGRAME
% COMPSEG = 501;  %NUMBER OF INTERVALS FOR THE SIGMA PROFILE FROM DMOL3
EPS = 3.667;  %(LIN AND SANDLER USE A CONSTANT FPOL WHICH YEILDS EPS=3.68)
COORD = 10.0;   %(KLAMT USED 7.2)
SIGMAHB = 0.0084; % No need to optimize the cuttoff parameter SIGMAHB
% SIGMAHB = PAR(5)*1e3;
CHB = 85580;      % Optimize for species that have the capacity for hydrogen bonding
% CHB = PAR(2);
% CHB = PAR(2)*1e-4;
COMP = 3;

FPOL = (EPS-1.0)/(EPS+0.5);
ALPHA = (0.3*AEFFPRIME^(1.5))/(EO);
ALPHAPRIME = FPOL*ALPHA;
Ces = (ALPHAPRIME/2.0);
% Ces = A + B/TEMP;
% DEFINE SYSTEM TEMPERATURE (K)
 SYSTEMP = TEMP;

% READ THE SIGMA PROFILES FOR THE PURE COMPONENTS
% ID = input('Enter ID # for Component 1 >>  ')
ID = ID1;
Comp_ID;
syscomp1 = syscomp;
% sigma = Sigma_Average(data);
ACOSMO(1)=acosmo;
VCOSMO(1)=vcosmo;
% global sigma

COUNTER(:,1) = sigma(:,1);
SIGMA (:,1)  = sigma(:,2);
```

```
% S1 = acosmo;
% S1 = S;

clear data acosmo vcosmo S NUMSEGMENT sigma

% ID = input('Enter ID # for Component 2 >>  ')
ID = ID2;
Comp_ID;
syscomp2 = syscomp;
% sigma = Sigma_Average(data);
ACOSMO(2)=acosmo;
VCOSMO(2)=vcosmo;

COUNTER(:,2) = sigma(:,1);
SIGMA(:,2)   = sigma(:,2);
% S2 = acosmo;
% S2 = S;
clear data acosmo vcosmo S NUMSEGMENT sigma

% ID = input('Enter ID # for Component 3 >>  ')
ID = ID3;
Comp_ID;
syscomp3 = syscomp;
% sigma = Sigma_Average(data);

ACOSMO(3)=acosmo;
VCOSMO(3)=vcosmo;

COUNTER(:,3) = sigma(:,1);
SIGMA(:,3)   = sigma(:,2);
% S3 = acosmo;
% S3 = S;
clear data acosmo vcosmo S NUMSEGMENT sigma


% MOLE FRACTIONS FOR TERNARY MIXTURE
x2 = 0.49999999999999;
x3 = 0.49999999999999;


%for m=1:length(x1) b
    FRAC2 = x2;
    FRAC3 = x3;
    FRAC1 = 1.0 - FRAC2 - FRAC3;


    %CALCULATE THE MIXTURE SIGMA PROFILE
        NUMER = FRAC1.*SIGMA(:,1) + FRAC2.*SIGMA(:,2)+ FRAC3.*SIGMA(:,3);
        DENOM = FRAC1.*ACOSMO(1) + FRAC2.*ACOSMO(2) + FRAC3.*ACOSMO(3);
        PROFILE = NUMER./DENOM;
%       disp( PROFILE )

     DELTAW = ones(COMPSEG,COMPSEG);

    for I = 1:COMPSEG
        for K = 1:COMPSEG
            if (COUNTER(I)>=COUNTER(K)) ;
```

```
                SIGMAACC = COUNTER(I);
                SIGMADON = COUNTER(K);
            end
            if (COUNTER(I)<COUNTER(K));
                SIGMADON = COUNTER(I);
                SIGMAACC = COUNTER(K);
            end

            DELTAW(I,K) = C1*Ces*(COUNTER(I)+COUNTER(K))^2.0 + C2*CHB *  ...
                max([0.0,(SIGMAACC - SIGMAHB)])*min([0.0,(SIGMADON + SIGMAHB)]) +
Cne;
% DELTAW(I,K) = Ces*(COUNTER(I)+COUNTER(K))^2.0 + C2*CHB *  ...
%                 max([0.0,(SIGMAACC - SIGMAHB)])*min([0.0,(SIGMADON + SIGMAHB)]) +
Cne;
        end
    end

    % !ITERATION FOR SEGMENT ACTIVITY COEF. (MIXTURE)
    CONVERG = ones(COMPSEG,1);
    SEGGAMMA =ones(COMPSEG,1);
    while (max(CONVERG) >= 0.000001)
        SEGGAMMAOLD = SEGGAMMA;
        for I = 1:COMPSEG
            SUMMATION = 0.0;
            for K = 1:COMPSEG
                SUMMATION = SUMMATION + PROFILE(K)* SEGGAMMAOLD(K) * ...
                    exp(-DELTAW(I,K)/(RGAS*SYSTEMP));
            end
            SEGGAMMA(I)=exp(-log(SUMMATION));
            SEGGAMMA(I)=(SEGGAMMA(I)+SEGGAMMAOLD(I))/2.0;
        end

        for I=1:COMPSEG
            CONVERG(I)=abs((SEGGAMMA(I)-SEGGAMMAOLD(I))/SEGGAMMAOLD(I));
        end
    end



    %!ITERATION FOR SEGMENT ACITIVITY COEF (PURE SPECIES)

    for L = 1:COMP
%         CONPR=1.0;
        SEGGAMMAOLDPR=ones(COMPSEG,COMP);
        SEGGAMMAPR=ones(COMPSEG,COMP);
        CONPR=ones(COMPSEG,COMP);
%         SEGGAMMAPR (:,L) = 1.0;
        while (max(CONPR) >=0.000001)
            SEGGAMMAOLDPR (:,L) = SEGGAMMAPR (:,L);
            for I = 1:COMPSEG
                SUMMATION = 0.0;
                for K = 1:COMPSEG
                    SUMMATION = SUMMATION + (SIGMA(K,L)/ACOSMO(L))*SEGGAMMAOLDPR(K,L)
* ...
                        exp(-DELTAW(I,K)/(RGAS*SYSTEMP));
                end
                SEGGAMMAPR(I,L)=exp(-log(SUMMATION));
```

```
                SEGGAMMAPR(I,L)=(SEGGAMMAPR(I,L)+SEGGAMMAOLDPR(I,L))/2.0;
            end
            for I=1:COMPSEG
                CONPR(I,L)=abs((SEGGAMMAPR(I,L)-
SEGGAMMAOLDPR(I,L))/SEGGAMMAOLDPR(I,L));
            end

        end
    end

    % !THE STAVERMAN-GUGGENHEIM EQUATION
    RNORM = VCOSMO./VNORM;
    QNORM = ACOSMO./ANORM;

    BOTTHETA = FRAC1*QNORM(1) + FRAC2*QNORM(2)+ FRAC3*QNORM(3);
    BOTPHI = FRAC1*RNORM(1) + FRAC2*RNORM(2)+ FRAC3*RNORM(3);

    THETA1 = (FRAC1*QNORM(1))/BOTTHETA;
%     THETA2 = (FRAC2*QNORM(2))/BOTTHETA;
%     THETA3 = (FRAC3*QNORM(3))/BOTTHETA;

    PHI1 = (FRAC1*RNORM(1))/BOTPHI;
%     PHI2 = (FRAC2*RNORM(2))/BOTPHI;
%     PHI3 = (FRAC3*RNORM(3))/BOTPHI;

    L1 = (COORD/2.0)*(RNORM(1)-QNORM(1))-(RNORM(1)-1.0);
    L2 = (COORD/2.0)*(RNORM(2)-QNORM(2))-(RNORM(2)-1.0);
    L3 = (COORD/2.0)*(RNORM(3)-QNORM(3))-(RNORM(3)-1.0);

    % !GAMMASG1 GAMMASG2 AND GAMMASG3 ARE ACTUALLY LNGAMMASG
    GAMMASG1 = log(PHI1/FRAC1)+(COORD/2)*QNORM(1)*log(THETA1/PHI1)+L1-(PHI1/FRAC1)*
...
        (FRAC1*L1 + FRAC2*L2 + FRAC3*L3);
%     GAMMASG2 = log(PHI2/FRAC2)+(COORD/2)*QNORM(2)*log(THETA2/PHI2)+L2-(PHI2/FRAC2)*
...
%         (FRAC1*L1 + FRAC2*L2 + FRAC3*L3);
%     GAMMASG3 = log(PHI3/FRAC3)+(COORD/2)*QNORM(3)*log(THETA3/PHI3)+L3-(PHI3/FRAC3)*
...
%         (FRAC1*L1 + FRAC2*L2 + FRAC3*L3);

    % !CALCULATION OF GAMMAS
    SUMGAMMA1 = 0.0;
%     SUMGAMMA2 = 0.0;
%     SUMGAMMA3 = 0.0;
    for I = 1:COMPSEG
        SUMGAMMA1 = SUMGAMMA1
+((SIGMA(I,1)/AEFFPRIME)*(log(SEGGAMMA(I)/(SEGGAMMAPR(I,1)))));
%         SUMGAMMA2 = SUMGAMMA2
+((SIGMA(I,2)/AEFFPRIME)*(log(SEGGAMMA(I)/(SEGGAMMAPR(I,2)))));
%         SUMGAMMA3 = SUMGAMMA3
+((SIGMA(I,3)/AEFFPRIME)*(log(SEGGAMMA(I)/(SEGGAMMAPR(I,3)))));

    end

%     GAMMAX  = exp(SUMGAMMA1 + GAMMASG1);
    GAMMA1  = exp(SUMGAMMA1 + GAMMASG1);
%     GAMMA2 = exp(SUMGAMMA2 + GAMMASG2);
```

```
%     GAMMA3 = exp(SUMGAMMA3 + GAMMASG3);

% LNGAMMA1 = log(GAMMAX) - log(D);
% LNGAMMA1 = log(GAMMAX);
% GAMMA1 = exp(LNGAMMA1);
%     LNGAMMA1 = log(GAMMA1);
%     LNGAMMA2 = log(GAMMA2);
%     LNGAMMA3 = log(GAMMA3);
%
%
%
%     Gex_RT = FRAC1*LNGAMMA1 + FRAC2*LNGAMMA2 + FRAC3*LNGAMMA3 + ...
%         FRAC1*log(FRAC1)+FRAC2*log(FRAC2)+ FRAC3*log(FRAC3);
% Gex_XXRT = A+B*(FRAC1-FRAC2)+C*(FRAC1-FRAC2)^2; % Redlich/Kister
% Gex_XXRT = A+B*(2*FRAC1-1); % Margules
% Gex_XXRT = ((A-B)*(A+B))/((A-B)*FRAC1)+((A+B)*FRAC2)); % Van Lar
% Gex_XXRT = A + B/TEMP; %Van't Hoff

% GAMMA_E = exp(Gex_XXRT);
% GAMMA_E = Gex_XXRT; %Van't Hoff
% D = Jacobian(Gex_RT,FRAC1,FRAC2,FRAC3);
% LNGAMMAX = log(GAMMA1) + log(D);
% GAMMAX = exp(LNGAMMAX);

%     result = [ FRAC1,GAMMA1, GAMMA2, GAMMA3, LNGAMMA1, LNGAMMA2, LNGAMMA3, Gex_RT];
%         result = [ FRAC1,GAMMA1, GAMMA2, GAMMA3, Gex_RT];


 IDAC(JJ) = m*GAMMA1;
% IDAC(JJ) = m*(GAMMA1) + GAMMA_E;
end
```

D.6 Data File for Optimization (Matlab File)

```
% % TEMP  SOLUTE_ID  CATION_ID  ANION_ID  IDAC_EXP
data2=[
    %-------------------------------------------------------------------
    %-----------------------VALIDATION DATA SET---------------------
    %-------------------------------------------------------------------

%         318.1500   18.0000  699.0000  850.0000    0.9400    0.9306    0.0099
90.6570   95.4437
%         323.1500   18.0000  699.0000  850.0000    0.9500    0.9209    0.0306
85.1206   88.6007
%         323.1500   18.0000  699.0000  850.0000    0.9500    0.9209    0.0306
85.1206   88.6007
%         333.1500   18.0000  699.0000  850.0000    0.9700    0.9026    0.0695
75.3622   76.6929
%         343.1500   18.0000  699.0000  850.0000    0.9800    0.8856    0.0963
67.0822   67.4512
%         333.1500   32.0000  699.0000  850.0000    0.5600    0.6175    0.1027
8.1011   13.4662
%         343.1500   32.0000  699.0000  850.0000    0.5700    0.6099    0.0699
7.7445   12.5868
%         353.1500   89.0000  699.0000  850.0000    1.7200    1.3550    0.2122
82.9631   47.2344
%         353.1500   92.0000  699.0000  850.0000    1.7300    1.2021    0.3052
52.5482   29.3747
%         318.1500   19.0000   59.0000  845.0000    2.4600    2.2578    0.0822
123.7797   49.3170
%         323.1500   19.0000   59.0000  845.0000    2.4700    2.2158    0.1029
117.5804   46.6034
%         333.1500   19.0000   59.0000  845.0000    2.4700    2.1369    0.1349
106.4252   42.0871
%         343.1500   19.0000   59.0000  845.0000    2.4800    2.0638    0.1678
96.7029   37.9931
%         353.1500   19.0000   59.0000  845.0000    2.4900    1.9961    0.1984
88.1882   34.4170
%         318.1500   32.0000   59.0000  845.0000    0.7000    0.9629    0.3756
1.8957    1.7082
%         323.1500   32.0000   59.0000  845.0000    0.7300    0.9655    0.3226
1.9658    1.6929
%         333.1500   32.0000   59.0000  845.0000    0.7800    0.9695    0.2429
2.1028    1.6959
%         343.1500   32.0000   59.0000  845.0000    0.8300    0.9719    0.1710
2.2347    1.6924
%         353.1500   32.0000   59.0000  845.0000    0.8900    0.9730    0.0933
2.3609    1.6527
%         318.1500   39.0000   59.0000  845.0000    4.4800    3.2124    0.2829
173.4382   37.7139
%         323.1500   39.0000   59.0000  845.0000    4.4600    3.1424    0.2954
165.2794   36.0582
%         333.1500   39.0000   59.0000  845.0000    4.4800    3.0111    0.3279
150.4571   32.5842
%         343.1500   39.0000   59.0000  845.0000    4.4100    2.8903    0.3446
137.3837   30.1528
%         353.1500   39.0000   59.0000  845.0000    4.3800    2.7790    0.3655
125.8093   27.7236
```

```
%         318.1500   94.0000   59.0000  845.0000    4.5100    3.9994    0.1132
42.7885    8.4875
%         323.1500   94.0000   59.0000  845.0000    4.5000    3.9090    0.1313
41.8921    8.3094
%         333.1500   94.0000   59.0000  845.0000    4.4800    3.7394    0.1653
40.1575    7.9637
%         343.1500   94.0000   59.0000  845.0000    4.4800    3.5835    0.2001
38.4998    7.5937
%         353.1500   94.0000   59.0000  845.0000    4.4600    3.4397    0.2288
36.9176    7.2775
%-----------------------------------------------------------------
%-------Other Validation Data Set-----------------------------------------------------
-------
%-----------------------------------------------------------------
%     323.15 44     699    850    15.40
%     323.15 17     699    850    2.41
%     323.15 18     699    850    0.95
%     323.15 37     699    850    22.40
%     333.15 44     699    850    14.70
%     333.15 17     699    850    2.45
%     333.15 32     699    850    0.56
%     333.15 18     699    850    0.97
%     333.15 37     699    850    20.90
%     343.15 44     699    850    14.00
%     343.15 37     699    850    19.70
%     343.15 120    699    850    10.60
%     343.15 15     699    850    27.40
%     353.15 17     699    850    2.52
%     353.15 92     699    850    1.73
%     353.15 89     699    850    1.72
%     313.15 30     699    852    0.95
%     323.15 30     699    852    0.92
%     318.15 29     699    850    1.53
%     318.15 20     699    850    1.55
%     318.15 30     699    850    1.32
%     318.15 27     699    850    1.03
%     323.15 29     699    850    1.46
%     323.15 20     699    850    1.48
%     323.15 30     699    850    1.27
%     323.15 27     699    850    0.99
%     333.15 29     699    850    1.34
%     333.15 20     699    850    1.35
%     333.15 30     699    850    1.17
%     333.15 27     699    850    0.93
%     343.15 29     699    850    1.24
%     343.15 20     699    850    1.25
%     343.15 30     699    850    1.09
%     343.15 27     699    850    0.88
%     353.15 29     699    850    1.15
%     353.15 20     699    850    1.16
%     353.15 30     699    850    1.02
%     353.15 27     699    850    0.83
%     298.15 30     699    849    0.60
%     298.15 27     699    849    0.33
%     308.15 30     699    849    0.59
%     318.15 30     699    849    0.59
%     328.15 30     699    849    0.58
```

```
%     323.15 30     59     844    0.57
%     333.15 30     59     844    0.60
%     343.15 30     59     844    0.65
%     353.15 30     59     844    0.70
%     318.15 44     59     845    374.00
%     318.15 39     59     845    4.48
%     318.15 17     59     845    34.60
%     318.15 19     59     845    2.46
%     318.15 22     59     845    0.86
%     318.15 94     59     845    4.51
%     318.15 12     59     845    123.00
%     318.15 32     59     845    0.70
%     318.15 18     59     845    7.32
%     318.15 92     59     845    19.10
%     318.15 37     59     845    637.00
%     318.15 120    59     845    211.00
%     318.15 89     59     845    20.80
%     318.15 15     59     845    1016.00
%     318.15 56     59     845    5.37
%     318.15 99     59     845    2.04
%     318.15 93     59     845    9.41
%     323.15 44     59     845    356.00
%     323.15 39     59     845    4.46
%     323.15 17     59     845    33.80
%     323.15 19     59     845    2.47
%     323.15 22     59     845    0.87
%     323.15 94     59     845    4.50
%     323.15 12     59     845    115.00
%     323.15 32     59     845    0.73
%     323.15 18     59     845    7.29
%     323.15 92     59     845    18.80
%     323.15 37     59     845    596.00
%     323.15 120    59     845    198.00
%     323.15 89     59     845    20.50
%     323.15 15     59     845    949.00
%     323.15 56     59     845    5.33
%     323.15 99     59     845    2.06
%     323.15 93     59     845    9.37
%     333.15 44     59     845    325.00
%     333.15 39     59     845    4.48
%     333.15 17     59     845    32.60
%     333.15 19     59     845    2.47
%     333.15 22     59     845    0.89
%     333.15 94     59     845    4.48
%     333.15 12     59     845    103.00
%     333.15 32     59     845    0.78
%     333.15 18     59     845    7.22
%     333.15 92     59     845    18.30
%     333.15 37     59     845    523.00
%     333.15 120    59     845    177.00
%     333.15 89     59     845    19.90
%     333.15 15     59     845    839.00
%     333.15 56     59     845    5.24
%     333.15 99     59     845    2.11
%     333.15 93     59     845    9.23
%     343.15 44     59     845    300.00
%     343.15 39     59     845    4.41
```

```
%     343.15 17     59     845    31.80
%     343.15 19     59     845    2.48
%     343.15 22     59     845    0.90
%     343.15 94     59     845    4.48
%     343.15 12     59     845    93.20
%     343.15 32     59     845    0.83
%     343.15 18     59     845    7.17
%     343.15 92     59     845    17.80
%     343.15 37     59     845    471.00
%     343.15 120    59     845    160.00
%     343.15 89     59     845    19.30
%     343.15 15     59     845    752.00
%     343.15 56     59     845    5.18
%     343.15 99     59     845    2.16
%     343.15 93     59     845    9.12
%     353.15 44     59     845    277.00
%     353.15 39     59     845    4.38
%     353.15 17     59     845    30.90
%     353.15 19     59     845    2.49
%     353.15 22     59     845    0.91
%     353.15 94     59     845    4.46
%     353.15 12     59     845    84.30
%     353.15 32     59     845    0.89
%     353.15 18     59     845    7.12
%     353.15 92     59     845    17.30
%     353.15 37     59     845    422.00
%     353.15 120    59     845    147.00
%     353.15 89     59     845    18.80
%     353.15 15     59     845    676.00
%     353.15 56     59     845    5.10
%     353.15 99     59     845    2.20
%     353.15 93     59     845    9.00
%     318.15 29     59     845    0.80
%     318.15 20     59     845    0.97
%     318.15 30     59     845    0.51
%     318.15 27     59     845    0.24
%     323.15 29     59     845    0.79
%     323.15 20     59     845    0.96
%     323.15 30     59     845    0.51
%     323.15 27     59     845    0.24
%     333.15 29     59     845    0.77
%     333.15 20     59     845    0.93
%     333.15 30     59     845    0.50
%     333.15 27     59     845    0.24
%     343.15 29     59     845    0.75
%     343.15 20     59     845    0.91
%     343.15 30     59     845    0.50
%     343.15 27     59     845    0.24
%     353.15 29     59     845    0.74
%     353.15 20     59     845    0.90
%     353.15 30     59     845    0.49
%     353.15 27     59     845    0.25
%     308.15 29     59     845    0.76
%     308.15 30     59     845    0.49
%     308.15 27     59     845    0.22
%     318.15 29     59     845    0.75
%     318.15 30     59     845    0.48
```

```
%     318.15 27     59     845    0.23
%     318.15 43     59     845    0.07
%     328.15 29     59     845    0.74
%     328.15 30     59     845    0.48
%     328.15 27     59     845    0.23
%     328.15 43     59     845    0.08
%     338.15 29     59     845    0.72
%     338.15 30     59     845    0.47
%     338.15 27     59     845    0.23
%     338.15 43     59     845    0.08
%     348.15 29     59     845    0.72
%     348.15 30     59     845    0.47
%     348.15 27     59     845    0.23
%     348.15 43     59     845    0.08
%     358.15 29     59     845    0.71
%     358.15 30     59     845    0.47
%     358.15 27     59     845    0.23
%     323.00 29     63     846    0.96
%     323.00 20     63     846    1.06
%     323.00 30     63     846    0.78
%     323.00 27     63     846    0.47
%     343.00 29     63     846    0.90
%     363.00 29     63     846    0.90
%     363.00 20     63     846    1.06
%     363.00 30     63     846    0.72
%     363.00 27     63     846    0.46
%     303.15 20     65     846    0.44
%     303.15 30     65     846    0.38
%     303.15 27     65     846    0.26
%     313.15 29     65     846    0.41
%     313.15 20     65     846    0.43
%     313.15 30     65     846    0.37
%     313.15 27     65     846    0.26
%     323.15 29     65     846    0.40
%     323.15 20     65     846    0.43
%     323.15 30     65     846    0.35
%     323.15 27     65     846    0.25
%     333.15 29     65     846    0.38
%     333.15 20     65     846    0.42
%     333.15 30     65     846    0.34
%     333.15 27     65     846    0.24
%     343.15 29     65     846    0.37
%     343.15 20     65     846    0.41
%     343.15 30     65     846    0.33
%     343.15 27     65     846    0.23
%     353.15 29     65     846    0.36
%     353.15 20     65     846    0.41
%     353.15 30     65     846    0.31
%     353.15 27     65     846    0.23
%     363.15 29     65     846    0.35
%     363.15 20     65     846    0.40
%     363.15 30     65     846    0.30
%     363.15 27     65     846    0.22
%     318.15 29     59     846    1.77
%     318.15 20     59     846    1.97
%     318.15 30     59     846    1.14
%     318.15 27     59     846    0.56
```

```
%     323.15 29     59     846    1.73
%     323.15 20     59     846    1.92
%     323.15 30     59     846    1.11
%     323.15 27     59     846    0.56
%     333.15 29     59     846    1.66
%     333.15 20     59     846    1.84
%     333.15 30     59     846    1.08
%     333.15 27     59     846    0.55
%     343.15 29     59     846    1.60
%     343.15 20     59     846    1.77
%     343.15 30     59     846    1.04
%     343.15 27     59     846    0.55
%     353.15 29     59     846    1.55
%     353.15 20     59     846    1.72
%     353.15 30     59     846    1.02
%     353.15 27     59     846    0.54
%     303.15 29     63     846    0.77
%     303.15 30     63     846    0.56
%     303.15 27     63     846    0.32
%     313.15 29     63     846    0.73
%     313.15 30     63     846    0.54
%     313.15 27     63     846    0.32
%     323.15 29     63     846    0.71
%     323.15 30     63     846    0.53
%     323.15 27     63     846    0.32
%     333.15 29     63     846    0.69
%     333.15 30     63     846    0.52
%     333.15 27     63     846    0.31
%     343.15 29     63     846    0.67
%     343.15 30     63     846    0.51
%     343.15 27     63     846    0.31
%     353.15 29     63     846    0.66
%     353.15 30     63     846    0.51
%     353.15 27     63     846    0.30
%     363.15 29     63     846    0.65
%     363.15 30     63     846    0.51
%     363.15 27     63     846    0.30
%     298.15 30     58     849    0.70
%     298.15 27     58     849    0.38
%     308.15 30     58     849    0.67
%     318.15 30     58     849    0.65
%     328.15 30     58     849    0.63
%     298.15 30     699    849    0.60
%     298.15 27     699    849    0.33
%     308.15 30     699    849    0.59
%     318.15 30     699    849    0.59
%     328.15 30     699    849    0.58
%     318.15 44     699    850    15.80
%     318.15 17     699    850    2.39
%     318.15 18     699    850    0.94
%     318.15 37     699    850    23.20
%     323.15 44     699    850    15.40
%     323.15 17     699    850    2.41
%     323.15 18     699    850    0.95
%     323.15 37     699    850    22.40
%     333.15 44     699    850    14.70
%     333.15 17     699    850    2.45
```

```
%     333.15 32     699    850    0.56
%     333.15 18     699    850    0.97
%     333.15 37     699    850    20.90
%     343.15 44     699    850    14.00
%     343.15 17     699    850    2.48
%     343.15 32     699    850    0.57
%     343.15 18     699    850    0.98
%     343.15 37     699    850    19.70
%     343.15 120    699    850    10.60
%     343.15 15     699    850    27.40
%     353.15 17     699    850    2.52
%     353.15 92     699    850    1.73
%     353.15 89     699    850    1.72
%     313.15 29     59     850    1.62
%     313.15 20     59     850    1.63
%     313.15 30     59     850    1.30
%     313.15 27     59     850    0.92
%     323.15 29     59     850    1.55
%     323.15 20     59     850    1.56
%     323.15 30     59     850    1.25
%     323.15 27     59     850    0.89
%     333.15 29     59     850    1.42
%     333.15 20     59     850    1.43
%     333.15 30     59     850    1.15
%     333.15 27     59     850    0.84
%     343.15 29     59     850    1.31
%     343.15 20     59     850    1.32
%     343.15 30     59     850    1.07
%     343.15 27     59     850    0.80
%     353.15 29     59     850    1.22
%     353.15 20     59     850    1.23
%     353.15 30     59     850    1.00
%     353.15 27     59     850    0.76
%     318.15 29     699    850    1.53
%     318.15 20     699    850    1.55
%     318.15 30     699    850    1.32
%     318.15 27     699    850    1.03
%     323.15 29     699    850    1.46
%     323.15 20     699    850    1.48
%     323.15 30     699    850    1.27
%     323.15 27     699    850    0.99
%     333.15 29     699    850    1.34
%     333.15 20     699    850    1.35
%     333.15 30     699    850    1.17
%     333.15 27     699    850    0.93
%     343.15 29     699    850    1.24
%     343.15 20     699    850    1.25
%     343.15 30     699    850    1.09
%     343.15 27     699    850    0.88
%     353.15 29     699    850    1.15
%     353.15 20     699    850    1.16
%     353.15 30     699    850    1.02
%     353.15 27     699    850    0.83
%     328.15 30     59     851    0.37
%     328.15 27     59     851    0.22
%     338.15 27     59     851    0.22
%     303.45 42     63     852    14.38
```

```
%     303.45 50     63     852    10.08
%     313.15 41     63     852    21.32
%     313.15 50     63     852    9.69
%     313.36 42     63     852    14.00
%     323.14 41     63     852    20.57
%     323.14 42     63     852    13.51
%     323.14 44     63     852    30.61
%     323.15 50     63     852    9.48
%     333.14 42     63     852    12.99
%     333.15 41     63     852    19.92
%     333.15 44     63     852    29.28
%     333.15 50     63     852    9.18
%     333.15 88     63     852    24.79
%     303.14 41     66     852    11.20
%     313.15 41     66     852    10.85
%     323.15 41     66     852    10.60
%     323.15 44     66     852    14.58
%     333.14 41     66     852    10.40
%     333.14 44     66     852    14.28
%     303.17 42     63     852    14.29
%     313.13 41     63     852    21.25
%     313.15 42     63     852    13.82
%     313.15 50     63     852    9.55
%     323.15 42     63     852    13.47
%     323.15 50     63     852    9.34
%     323.16 41     63     852    20.25
%     323.16 57     63     852    17.46
%     333.16 41     63     852    19.74
%     333.16 44     63     852    28.99
%     333.18 42     63     852    12.95
%     333.18 50     63     852    9.06
%     333.22 57     63     852    16.75
%     303.18 42     66     852    7.40
%     303.18 50     66     852    4.62
%     313.15 42     66     852    7.23
%     313.15 50     66     852    4.58
%     313.17 41     66     852    10.60
%     323.15 41     66     852    10.40
%     323.16 42     66     852    7.03
%     323.16 50     66     852    4.54
%     333.15 42     66     852    6.86
%     333.15 50     66     852    4.51
%     333.18 41     66     852    10.07
%     333.18 44     66     852    13.72
%     303.13 42     65     852    4.68
%     313.13 42     65     852    4.61
%     323.14 41     65     852    5.97
%     323.16 42     65     852    4.57
%     333.12 41     65     852    5.89
%     333.12 44     65     852    7.66
%     333.16 42     65     852    4.53
%     313.15 30     699    852    0.95
%     323.15 30     699    852    0.92
%     303.15 25     63     852    1.97
%     303.15 87     63     852    1.84
%     303.15 20     63     852    1.45
%     303.15 30     63     852    1.14
```

```
%     313.15 28     63     852    1.85
%     313.15 25     63     852    1.82
%     313.15 87     63     852    1.74
%     313.15 20     63     852    1.37
%     313.15 27     63     852    0.68
%     323.15 28     63     852    1.78
%     323.15 26     63     852    2.34
%     323.15 87     63     852    1.64
%     323.15 27     63     852    0.67
%     333.15 28     63     852    1.71
%     333.15 26     63     852    2.16
%     333.15 87     63     852    1.51
%     333.15 27     63     852    0.65
%     343.15 28     63     852    1.57
%     343.15 87     63     852    1.38
%     343.15 27     63     852    0.65
%     353.15 25     63     852    1.49
%     353.15 87     63     852    1.29
%     353.15 27     63     852    0.63
%     363.15 25     63     852    1.43
%     363.15 87     63     852    1.20
%     298.15 30     63     852    1.07
%     308.15 28     63     852    1.66
%     308.15 29     63     852    1.27
%     308.15 30     63     852    1.01
%     318.15 28     63     852    1.57
%     318.15 29     63     852    1.20
%     318.15 30     63     852    0.96
%     328.15 28     63     852    1.49
%     328.15 29     63     852    1.14
%     328.15 30     63     852    0.91
%     338.15 28     63     852    1.42
%     338.15 29     63     852    1.09
%     338.15 30     63     852    0.87
%     348.15 28     63     852    1.35
%     348.15 29     63     852    1.04
%     348.15 30     63     852    0.83
%     358.15 28     63     852    1.29
%     358.15 30     63     852    0.80
%     368.15 28     63     852    1.23
%-------------------------------------------------------------------
%------------------------OPTIMIZATION DATA SET----------------------
%-------------------------------------------------------------------
            313.15           94           58           70        1.639
            323.15           94           58           70        1.645
            333.15           94           58           70        1.648
            343.15           94           58           70        1.652
            313.15           96           58           70         1.98
            323.15           96           58           70        2.019
            333.15           96           58           70        2.053
            343.15           96           58           70        2.084
            293.15           94           60           72         1.33
            303.15           94           60           72         1.34
            313.15           94           60           72         1.35
            323.15           94           60           72         1.36
            333.15           94           60           72         1.37
            293.15           93           60           72            2
```

303.15	93	60	72	2.01
313.15	93	60	72	2.02
323.15	93	60	72	2.04
293.15	94	59	71	2.7
303.15	94	59	71	2.73
313.15	94	59	71	2.76
323.15	94	59	71	2.8
333.15	94	59	71	2.83
313.76	19	58	70	0.908
323.02	19	58	70	0.914
333.25	19	58	70	0.919
343.58	19	58	70	0.921
313.71	22	58	70	0.58
322.93	22	58	70	0.577
333.23	22	58	70	0.57
343.57	22	58	70	0.564
313.68	32	58	70	0.748
323.02	32	58	70	0.757
333.38	32	58	70	0.766
343.78	32	58	70	0.772
313.73	33	58	70	0.732
323.05	33	58	70	0.768
333.46	33	58	70	0.8
343.96	33	58	70	0.832
313.15	33	59	72	0.972
323.15	33	59	72	0.989
333.15	33	59	72	1.011
343.15	33	59	72	1.029
313.15	32	59	72	0.891
323.15	32	59	72	0.882
333.15	32	59	72	0.869
343.15	32	59	72	0.862
313.15	18	59	72	0.886
323.15	18	59	72	0.9
333.15	18	59	72	0.91
343.15	18	59	72	0.924
313.15	19	59	72	0.399
323.15	19	59	72	0.406
333.15	19	59	72	0.412
343.15	19	59	72	0.415
313.15	22	59	72	0.435
323.15	22	59	72	0.429
333.15	22	59	72	0.425
343.15	22	59	72	0.419
313.15	91	59	72	2.396
323.15	91	59	72	2.414
313.15	93	59	72	1.735
323.15	93	59	72	1.735
333.15	93	59	72	1.762
343.15	93	59	72	1.776
313.15	94	59	72	1.199
323.15	94	59	72	1.179
333.15	94	59	72	1.189
343.15	94	59	72	1.181
313.15	96	59	72	1.664
323.15	96	59	72	1.668
333.15	96	59	72	1.668

343.15	96	59	72	1.68
313.15	19	62	72	0.462
323.15	19	62	72	0.464
333.15	19	62	72	0.468
343.15	19	62	72	0.469
313.15	22	62	72	0.462
323.15	22	62	72	0.453
333.15	22	62	72	0.449
343.15	22	62	72	0.44
313.15	32	62	72	0.909
323.15	32	62	72	0.892
333.15	32	62	72	0.879
343.15	32	62	72	0.858
313.15	18	62	72	1.068
323.15	18	62	72	1.069
333.15	18	62	72	1.07
343.15	18	62	72	1.07
313.15	94	62	72	1.097
323.15	94	62	72	1.1
333.15	94	62	72	1.101
343.15	94	62	72	1.105
313.15	96	62	72	1.49
323.15	96	62	72	1.502
333.15	96	62	72	1.514
343.15	96	62	72	1.531
293.15	38	59	72	0.703
303.15	38	59	72	0.724
313.15	38	59	72	0.743
323.15	38	59	72	0.763
293.15	39	59	72	0.544
303.15	39	59	72	0.556
313.15	39	59	72	0.571
323.15	39	59	72	0.586
293.15	19	59	72	0.403
303.15	19	59	72	0.404
313.15	19	59	72	0.41
323.15	19	59	72	0.423
293.15	93	59	72	1.82
303.15	93	59	72	1.81
313.15	93	59	72	1.81
323.15	93	59	72	1.81
293.15	94	59	72	1.18
303.15	94	59	72	1.19
313.15	94	59	72	1.2
323.15	94	59	72	1.21
293.15	94	63	72	0.872
303.15	94	63	72	0.881
313.15	94	63	72	0.892
323.15	94	63	72	0.903
303.15	93	63	72	1.22
313.15	93	63	72	1.24
323.15	93	63	72	1.26
333.15	93	63	72	1.28
298.15	45	65	73	3.07
308.15	45	65	73	2.91
318.15	45	65	73	2.82
298.15	47	65	73	2.47

308.15	47	65	73	2.32
318.15	47	65	73	2.26
298.15	94	66	74	1.03
313.15	94	66	74	1.04
323.15	94	66	74	1.07
298.15	94	66	74	0.96
323.15	94	66	74	0.95
323.15	27	66	74	0.61
343.15	29	60	77	0.18
353.15	29	60	77	0.19
363.15	29	60	77	0.19
373.15	29	60	77	0.2
343.15	30	60	77	0.122
353.15	30	60	77	0.13
363.15	30	60	77	0.14
373.15	30	60	77	0.14
303.15	19	60	77	2.3
313.15	19	60	77	2.3
323.15	19	60	77	2.3
333.15	19	60	77	2.3
333.15	27	60	78	0.55
303.15	54	69	72	1.15
313.15	54	69	72	1.16
323.15	54	69	72	1.16
333.15	54	69	72	1.15
303.15	38	69	72	0.93
313.15	38	69	72	0.93
323.15	38	69	72	0.94
333.15	38	69	72	0.94
303.15	19	69	72	0.46
313.15	19	69	72	0.47
323.15	19	69	72	0.48
333.15	19	69	72	0.49
303.15	33	69	72	1.14
313.15	33	69	72	1.14
323.15	33	69	72	1.14
333.15	33	69	72	1.15
303.15	32	69	72	1.05
313.15	32	69	72	1.03
323.15	32	69	72	1.01
333.15	32	69	72	0.98
303.15	39	68	76	3.1
313.15	39	68	76	3.1
303.15	19	68	76	1.8
313.15	19	68	76	1.8
323.15	19	68	76	1.8
333.15	19	68	76	1.8
303.15	19	68	76	1.8
313.15	19	68	76	1.8
323.15	19	68	76	1.8
333.15	19	68	76	1.8
303.15	90	69	72	2.6
313.15	90	69	72	2.6
303.15	89	69	72	2.7
303.15	93	69	72	1.9
313.15	93	69	72	1.9
323.15	93	69	72	2

303.15	94	69	72	1.26
313.15	94	69	72	1.3
323.15	94	69	72	1.4
333.15	94	69	72	1.4
303.15	56	69	72	0.86
313.15	56	69	72	0.86
323.15	56	69	72	0.86
333.15	56	69	72	0.86
303.15	43	60	77	0.052
313.15	43	60	77	0.054
323.15	43	60	77	0.058
298.15	94	63	80	1.42
313.15	94	63	80	1.44
328.15	94	63	80	1.45
298.15	93	63	80	1.98
313.15	93	63	80	2.02
328.15	93	63	80	2.08
298.15	35	63	80	1.65
313.15	35	63	80	1.74
328.15	35	63	80	1.85
298.15	27	63	80	0.386
313.15	27	63	80	0.369
328.15	27	63	80	0.36
298.15	27	63	81	0.345
303.15	27	63	81	0.342
308.15	27	63	81	0.337
298.15	94	63	81	2.04
303.15	94	63	81	2.02
298.15	35	66	72	1.67
298.15	94	66	72	0.674
313.15	94	66	72	0.687
333.15	94	66	72	0.7
313.15	99	63	74	1.37
323.15	99	63	74	1.47
313.15	86	63	74	1.05
323.15	86	63	74	1.13
333.15	86	63	74	1.23
313.15	22	63	74	0.51
323.15	22	63	74	0.55
333.15	22	63	74	0.6
313.15	32	63	74	0.79
323.15	32	63	74	0.9
333.15	32	63	74	1.04
313.15	33	63	74	1.3
333.15	55	63	74	0.74
363.15	56	65	70	1.09
363.15	43	59	70	0.45
363.15	27	59	70	0.4
363.15	43	63	73	0.1
363.15	30	63	73	0.2
353.15	27	60	77	0.029
353.15	19	63	72	0.406
353.15	56	59	72	0.8
353.15	19	59	72	0.438
353.15	43	60	77	0.028
353.15	30	60	77	0.115
313.15	22	65	73	0.86

313.15	32	65	73	0.22
313.15	33	65	73	0.09
313.15	20	65	73	0.25
313.15	29	65	73	0.12
313.15	30	65	73	0.12
313.15	27	65	73	0.08
313.15	47	65	73	2.02
313.15	99	59	72	1.07
313.15	55	59	72	0.61
313.15	86	59	72	0.82
313.15	22	59	72	0.47
313.15	32	59	72	0.69
313.15	33	59	72	0.99
313.15	51	59	72	0.64
313.15	38	59	72	0.77
313.15	39	59	72	0.6
313.15	91	59	72	2.4
313.15	90	59	72	2.44
313.15	93	59	72	1.97
301.65	94	66	72	0.7785
306.95	94	66	72	0.776
312.25	94	66	72	0.776
322.75	94	66	72	0.777
322.85	94	66	72	0.773
333.25	94	66	72	0.777
343.75	94	66	72	0.769
301.75	33	66	72	0.67
301.85	33	66	72	0.67
312.25	33	66	72	0.68
312.45	33	66	72	0.68
322.85	33	66	72	0.69
323.05	33	66	72	0.7
333.45	33	66	72	0.71
343.95	33	66	72	0.72
301.75	107	66	72	1.11
312.25	107	66	72	1.1
322.85	107	66	72	1.08
333.35	107	66	72	1.06
343.55	107	66	72	1.05
354.05	107	66	72	1.03
364.45	107	66	72	1.01
374.95	107	66	72	0.99
301.75	19	66	72	0.352
302.25	19	66	72	0.352
312.25	19	66	72	0.357
322.85	19	66	72	0.362
333.35	19	66	72	0.366
343.85	19	66	72	0.371
354.25	19	66	72	0.375
301.8	94	59	71	2.98
312.3	94	59	71	2.94
323	94	59	71	2.88
333.5	94	59	71	2.79
343.9	94	59	71	2.69
354.4	94	59	71	2.59
288.15	27	65	81	0.405
298.15	27	65	81	0.38

313.15	27	65	81	0.37
343.55	110	66	72	1.11
354.05	110	66	72	1.07
364.45	110	66	72	1.02
374.95	110	66	72	0.97
385.35	110	66	72	0.92
395.95	110	66	72	0.9
323.1	19	59	71	1.64
333.6	19	59	71	1.63
343.9	19	59	71	1.61
365	19	59	71	1.56
375.4	19	59	71	1.54
386	19	59	71	1.5
288.15	94	65	81	1.33
298.15	94	65	81	1.395
313.15	94	65	81	1.36
301.75	109	64	72	0.84
312.25	109	64	72	0.8
322.75	109	64	72	0.79
343.55	109	64	72	0.77
354.15	109	64	72	0.76
322.75	94	64	72	1.3
333.35	94	64	72	1.26
343.55	94	64	72	1.26
354.05	94	64	72	1.22
364.45	94	64	72	1.2
301.75	22	64	72	0.52
312.45	22	64	72	0.5
322.95	22	64	72	0.49
333.35	22	64	72	0.47
343.75	22	64	72	0.46
301.65	116	64	72	0.58
312.25	116	64	72	0.57
322.75	116	64	72	0.54
333.25	116	64	72	0.53
343.55	116	64	72	0.52
374.95	110	64	72	1.6
385.45	110	64	72	1.48
395.95	110	64	72	1.36
307.05	93	66	72	1.04
312.35	93	66	72	1.04
322.85	93	66	72	1.06
333.35	93	66	72	1.06
343.85	93	66	72	1.08
312.25	22	66	72	0.456
322.85	22	66	72	0.446
333.35	22	66	72	0.434
343.85	22	66	72	0.426
354.25	22	66	72	0.413
333.15	115	66	72	1.2
343.55	115	66	72	1.21
354.05	115	66	72	1.23
364.45	115	66	72	1.24
374.95	115	66	72	1.26
343.65	118	66	72	1.39
354.15	118	66	72	1.35
364.65	118	66	72	1.29

375.15	118	66	72	1.25
385.65	118	66	72	1.2
312.4	27	59	71	0.41
323	27	59	71	0.4
333.4	27	59	71	0.39
343.8	27	59	71	0.38
354.2	27	59	71	0.36
333.5	116	59	71	1.94
343.9	116	59	71	1.9
354.4	116	59	71	1.84
364.8	116	59	71	1.8
375.2	116	59	71	1.74
303.15	93	63	70	2.913
303.15	94	63	70	1.739
313.15	94	63	70	1.758
323.15	94	63	70	1.77
333.15	94	63	70	1.798
343.15	94	63	70	1.83
313.15	96	63	70	2.293
323.15	96	63	70	2.339
333.15	96	63	70	2.411
343.15	96	63	70	2.475
322.75	113	64	72	1.66
333.15	113	64	72	1.63
364.55	113	64	72	1.44
374.95	113	64	72	1.33
322.75	119	66	72	0.868
333.25	119	66	72	0.874
343.65	119	66	72	0.877
354.15	119	66	72	0.884
322.75	113	66	72	1.04
333.25	113	66	72	1.03
343.65	113	66	72	1.01
354.15	113	66	72	0.99
354.15	114	66	72	1.6
364.65	114	66	72	1.52
375.15	114	66	72	1.44
385.65	114	66	72	1.38
322.75	112	66	72	0.681
333.25	112	66	72	0.683
343.65	112	66	72	0.685
354.15	112	66	72	0.688
301.75	109	66	72	0.578
312.25	109	66	72	0.576
322.85	109	66	72	0.574
333.35	109	66	72	0.572
301.75	116	66	72	0.453
312.25	116	66	72	0.45
322.85	116	66	72	0.444
333.35	116	66	72	0.439
322.85	92	66	72	1.55
333.35	92	66	72	1.55
343.85	92	66	72	1.54
354.25	92	66	72	1.53
312.2	22	59	71	0.81
333.4	22	59	71	0.8
343.9	22	59	71	0.78

```
            354.3           22           59           71         0.77];

% [m,n]=size(data2);
% counter =0;
% Highest_IDAC = input('Enter Highest IDAC value >>  ');
% Lowest_IDAC = input('Enter Lowest IDAC value >>  ');
% for i=1:m;
%     if data2(i,5) <= Highest_IDAC
%         if data2(i,5) > Lowest_IDAC
%             TEMP=data2(i,1);
%             SOLUTE_ID=data2(i,2);
%             CATION_ID=data2(i,3);
%             ANION_ID=data2(i,4);
%             IDAC_EXP=data2(i,5);
%             counter = counter + 1;
%             result1(counter,:) = [TEMP SOLUTE_ID CATION_ID ANION_ID IDAC_EXP];
%         end
%     end
% end
% disp(result1)
% %
% data2=result1;
% Data_Points = length(data2)

% % FILTERING OF DATA WITH LOWEST RESIDUAL
% Highest_Residual = input('Enter Highest Residual Value Expected >>  ');
% [m,n]=size(res);
% counter =0;
% for i=1:m;
%     if abs(res(i,1)) < Highest_Residual
%         TEMP=data2(i,1);
%         SOLUTE_ID=data2(i,2);
%         CATION_ID=data2(i,3);
%         ANION_ID=data2(i,4);
%         IDAC_EXP=data2(i,5);
%         REF_RES = res(i,1);
%         counter = counter + 1;
%         result1(counter,:) = [TEMP SOLUTE_ID CATION_ID ANION_ID IDAC_EXP];
%         res1(counter,1) = REF_RES;
%     end
%
% end
% disp(result1)
%
% data2=result1;

XDATA = data2(:,1:4);
YDATA = data2(:,5);
NVARS = 2;
% par0 = Initial Parameter Values
par0 = [6.5285 79.53 66.69 1.8133e-3 1.2433 3.2563e-2];
% par0 = [87.199 153.92 10320 1.502e-3 1.2 0.680];

% lb = [0 0];
lb = [0 0 0 0 0 0];
ub = [inf inf inf inf inf inf];
% ub = [inf inf];
```

D.7 Validation Programme (Matlab)

```
clear all
clc

DataFile;
counter = 0;
% PAR = [6.5285 0.001813 1.2433 0.032563];
PAR_orig = [7.5 79.53 66.69 1 1 0.0];
PAR_optim_prelim = [87.199 153.92 10320 1.502e-3 1.2 0.680];
PAR_optim_main = [7.6492 236.61 3.11179 3.4153e-14 1.2775 0.050649];

data2;
[p,q] = size(data2);
tic
for i = 1:p
    TEMP = data2(i,1);
    SOLUTE_ID = data2(i,2);
    CAT_ID = data2(i,3);
    ANI_ID = data2(i,4);
    IDAC_EXPT = data2(i,5);
    INPUT_DATA = [TEMP,SOLUTE_ID,CAT_ID,ANI_ID,IDAC_EXPT];
    IDAC_ORIG = COSMO_SAC_TERNARY(PAR_orig,INPUT_DATA);
    IDAC_OPTIM_PRELIM = COSMO_SAC_TERNARY(PAR_optim_prelim,INPUT_DATA);
    IDAC_OPTIM_MAIN = COSMO_SAC_TERNARY(PAR_optim_main,INPUT_DATA);
    counter = counter + 1;
    RD_OPTIM_MAIN = 1/abs((IDAC_OPTIM_MAIN-IDAC_EXPT)/IDAC_EXPT);
    RD_OPTIM_PRELIM = abs((IDAC_OPTIM_PRELIM-IDAC_EXPT)/IDAC_EXPT);
%     MAE = (1/counter)*(abs(IDAC_OPTIM_MAIN-IDAC_EXPT));
% MAPE =
                        RD_ORIG = abs((IDAC_ORIG-IDAC_EXPT)/IDAC_EXPT);
    result1(counter,:) = [TEMP SOLUTE_ID CAT_ID ANI_ID IDAC_EXPT IDAC_ORIG RD_ORIG
IDAC_OPTIM_PRELIM RD_OPTIM_PRELIM IDAC_OPTIM_MAIN RD_OPTIM_MAIN];
end
toc
disp('  TEMP SOLUTE_ID CAT_ID ANI_ID IDAC_EXPT IDAC_ORIG RD_ORIG IDAC_OPTIM_PRELIM
RD_OPTIM_PRELIM IDAC_OPTIM_MAIN RD_OPTIM_MAIN')
disp(result1)
IDAC_EXPT = data2(:,5);
IDAC_ORIG = COSMO_SAC_TERNARY(PAR_orig,XDATA);
IDAC_OPTIM_MAIN = COSMO_SAC_TERNARY(PAR_optim_main,XDATA);
IDAC_OPTIM_PRELIM = COSMO_SAC_TERNARY(PAR_optim_prelim,XDATA);

figure(1)
plot(IDAC_ORIG,IDAC_EXPT,'o',IDAC_EXPT,IDAC_EXPT,'-')
legend('Original Model','Experimantal')
title(' Parity Plot for Experimental IDAC and Original Model IDAC')
xlabel(' Experimental IDAC');
ylabel(' Original Model IDAC')
grid;
figure(2)
plot(IDAC_OPTIM_MAIN,IDAC_EXPT,'O', IDAC_EXPT,IDAC_EXPT,'-')
legend('Optimized Model','Experimantal')
title(' Parity Plot for Experimental IDAC and Optimized Model IDAC')
xlabel(' Experimental IDAC')
ylabel(' Optimized Model IDAC')
grid;
```

```
figure(3)
plot(IDAC_OPTIM_PRELIM,IDAC_EXPT,'O', IDAC_EXPT,IDAC_EXPT,'-')
legend('Prelim Model','Experimantal')
title(' Parity Plot for Experimental IDAC and Prelim Model IDAC')
xlabel(' Experimental IDAC')
ylabel(' Prelim Model IDAC')
grid;

DataFile;
yfit = PAR_optim_main;
ydata = IDAC_EXPT;
YMODEL = IDAC_OPTIM_MAIN;
% YMODEL = IDAC_ORIG;
% YMODEL = IDAC_OPTIM_PRELIM;
PAR = PAR_optim_main;
YDATA = IDAC_EXPT;
[res, r2, r2adj, SSE, RMSE] = stat_data(PAR,YMODEL,YDATA)

% [std,varresid,r2,cor,vcv,varinf]=regdata(PAR_optim_main,YMODEL,YDATA,jac);

fileID = fopen('testdata.txt','w');
fprintf(fileID,'%6s\r\n','PAR_optim_main');
fprintf(fileID,'%12.4f',PAR_optim_main);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','r2');
fprintf(fileID,'%12.4f',r2);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','r2adj');
fprintf(fileID,'%12.4f',r2adj);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','res');
fprintf(fileID,'%12.4f',res);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','RMSE');
fprintf(fileID,'%12.4f',RMSE);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','SSE');
fprintf(fileID,'%12.4f',SSE);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
% fprintf(fileID,'%6s\r\n','exitflag');
% fprintf(fileID,'%12.0f',exitflag);
fprintf(fileID,'%6s\r\n','');
fprintf(fileID,'%6s\r\n','');
fclose(fileID);
```

D.8 COMPONENT ID MATLAB PROGRAMME FILE

```
switch ID
    case 10
        SOL_10;
        syscomp = 'SOL_10';
    case 11
        SOL_11;
        syscomp = 'SOL_11';
    case 12
        SOL_12;
        syscomp = 'SOL_12';
    case 13
        SOL_13;
        syscomp = 'SOL_13';
    case 14
        SOL_14;
        syscomp = 'SOL_14';
    case 15
        SOL_15;
        syscomp = 'SOL_15';
    case 16
        SOL_16;
        syscomp = 'SOL_16';
    case 17
        SOL_17;
        syscomp = 'SOL_17';
    case 18
        SOL_18;
        syscomp = 'SOL_18';
    case 19
        SOL_19;
        syscomp = 'SOL_19';
    case 20
        SOL_20;
        syscomp = 'SOL_20';
    case 21
        SOL_21;
        syscomp = 'SOL_21';
    case 22
        SOL_22;
        syscomp = 'SOL_22';
    case 23
        SOL_23;
        syscomp = 'SOL_23';
    case 24
        SOL_24;
        syscomp = 'SOL_24';
    case 25
        SOL_25;
        syscomp = 'SOL_25';
    case 26
        SOL_26;
        syscomp = 'SOL_26';
    case 27
        SOL_27;
        syscomp = 'SOL_27';
```

```
case 28
    SOL_28;
    syscomp = 'SOL_28';
case 29
    SOL_29;
    syscomp = 'SOL_29';
case 30
    SOL_30;
    syscomp = 'SOL_30';
case 31
    SOL_31;
    syscomp = 'SOL_31';
case 32
    SOL_32;
    syscomp = 'SOL_32';
case 33
    SOL_33;
    syscomp = 'SOL_33';
case 34
    SOL_34;
    syscomp = 'SOL_34';
case 35
    SOL_35;
    syscomp = 'SOL_35';
case 36
    SOL_36;
    syscomp = 'SOL_36';
case 37
    SOL_37;
    syscomp = 'SOL_37';
case 38
    SOL_38;
    syscomp = 'SOL_38';
case 39
    SOL_39;
    syscomp = 'SOL_39';
case 40
    SOL_40;
    syscomp = 'SOL_40';
case 41
    SOL_41;
    syscomp = 'SOL_41';
case 42
    SOL_42;
    syscomp = 'SOL_42';
case 43
    SOL_43;
    syscomp = 'SOL_43';
case 44
    SOL_44;
    syscomp = 'SOL_44';
case 45
    SOL_45;
    syscomp = 'SOL_45';
case 46
    SOL_46;
    syscomp = 'SOL_46';
```

```
case 47
    SOL_47;
    syscomp = 'SOL_47';
case 48
    SOL_48;
    syscomp = 'SOL_48';
case 49
    SOL_49;
    syscomp = 'SOL_49';
case 50
    SOL_50;
    syscomp = 'SOL_50';
case 51
    SOL_51;
    syscomp = 'SOL_51';
case 52
    SOL_52;
    syscomp = 'SOL_52';
case 53
    SOL_53;
    syscomp = 'SOL_53';
case 54
    SOL_54;
    syscomp = 'SOL_54';
case 55
    SOL_55;
    syscomp = 'SOL_55';
case 56
    SOL_56;
    syscomp = 'SOL_56';
case 57
    SOL_57;
    syscomp = 'SOL_57';
case 58
    CAT_58;
    syscomp = 'CAT_58';
case 59
    CAT_59;
    syscomp = 'CAT_59';
case 60
    CAT_60;
    syscomp = 'CAT_60';
case 61
    CAT_61;
    syscomp = 'CAT_61';
case 62
    CAT_62;
    syscomp = 'CAT_62';
case 63
    CAT_63;
    syscomp = 'CAT_63';
case 64
    CAT_64;
    syscomp = 'CAT_64';
case 65
    CAT_65;
    syscomp = 'CAT_65';
```

```
case 66
    CAT_66;
    syscomp = 'CAT_66';
case 67
    CAT_67;
    syscomp = 'CAT_67';
case 68
    CAT_68;
    syscomp = 'CAT_68';
case 69
    CAT_69;
    syscomp = 'CAT_69';
case 70
    ANI_70;
    syscomp = 'ANI_70';
case 71
    ANI_71;
    syscomp = 'ANI_71';
case 72
    ANI_72;
    syscomp = 'ANI_72';
case 73
    ANI_73;
    syscomp = 'ANI_73';
case 74
    ANI_74;
    syscomp = 'ANI_74';
case 75
    ANI_75;
    syscomp = 'ANI_75';
case 76
    ANI_76;
    syscomp = 'ANI_76';
case 77
    ANI_77;
    syscomp = 'ANI_77';
case 78
    ANI_78;
    syscomp = 'ANI_78';
case 79
    ANI_79;
    syscomp = 'ANI_79';
case 80
    ANI_80;
    syscomp = 'ANI_80';
case 81
    ANI_81;
    syscomp = 'ANI_81';
case 82
    ANI_82;
    syscomp = 'ANI_82';
case 83
    ANI_83;
    syscomp = 'ANI_83';
case 84
    ANI_84;
    syscomp = 'SOL_84';
```

```
case 85
    SOL_85;
    syscomp = 'SOL_85';
case 86
    SOL_86;
    syscomp = 'SOL_86';
case 87
    SOL_87;
    syscomp = 'SOL_87';
case 88
    SOL_88;
    syscomp = 'SOL_88';
case 89
    SOL_89;
    syscomp = 'SOL_89';
case 90
    SOL_90;
    syscomp = 'SOL_90';
case 91
    SOL_91;
    syscomp = 'SOL_91';
case 92
    SOL_92;
    syscomp = 'SOL_92';
case 93
    SOL_93;
    syscomp = 'SOL_93';
case 94
    SOL_94;
    syscomp = 'SOL_94';
case 95
    SOL_95;
    syscomp = 'SOL_95';
case 96
    SOL_96;
    syscomp = 'SOL_96';
case 97
    SOL_97;
    syscomp = 'SOL_97';
case 98
    SOL_98;
    syscomp = 'SOL_98';
case 99
    SOL_99;
    syscomp = 'SOL_99';
case 100
    SOL_100;
    syscomp = 'SOL_100';
case 101
    SOL_101;
    syscomp = 'SOL_101';
case 102
    SOL_102;
    syscomp = 'SOL_102';
case 103
    SOL_103;
    syscomp = 'SOL_103';
```

```
case 104
    SOL_104;
    syscomp = 'SOL_104';
case 105
    SOL_105;
    syscomp = 'SOL_105';
case 106
    SOL_106;
    syscomp = 'SOL_106';
case 107
    SOL_107;
    syscomp = 'SOL_107';
case 108
    SOL_108;
    syscomp = 'SOL_108';
case 109
    SOL_109;
    syscomp = 'SOL_109';
case 110
    SOL_110;
    syscomp = 'SOL_110';
case 111
    SOL_111;
    syscomp = 'SOL_111';
case 112
    SOL_112;
    syscomp = 'SOL_112';
case 113
    SOL_113;
    syscomp = 'SOL_113';
case 114
    SOL_114;
    syscomp = 'SOL_114';
case 115
    SOL_115;
    syscomp = 'SOL_115';
case 116
    SOL_116;
    syscomp = 'SOL_116';
case 117
    SOL_117;
    syscomp = 'SOL_117';
case 118
    SOL_118;
    syscomp = 'SOL_118';
case 119
    SOL_119;
    syscomp = 'SOL_119';
case 120
    SOL_120;
    syscomp = 'SOL_120';
case 121
    SOL_121;
    syscomp = 'SOL_121';
case 122
    SOL_122;
    syscomp = 'SOL_122';
```

```
    case 123
        SOL_123;
        syscomp = 'SOL_123';
    case 691
        CAT_691;
        syscomp = 'CAT_691';
    case 692
        CAT_692;
        syscomp = 'CAT_692';
    case 693
        CAT_693;
        syscomp = 'CAT_693';
    case 694
        CAT_694;
        syscomp = 'CAT_694';
    case 696
        CAT_696;
        syscomp = 'CAT_696';
    case 697
        CAT_697;
        syscomp = 'CAT_697';
    case 699
        CAT_699;
        syscomp = 'CAT_699';
    case 841
        ANI_841;
        syscomp = 'ANI_841';
    case 842
        ANI_842;
        syscomp = 'ANI_842';
    case 844
        ANI_844;
        syscomp = 'ANI_844';
    case 845
        ANI_845;
        syscomp = 'ANI_845';
    case 846
        ANI_846;
        syscomp = 'ANI_846';
    case 849
        ANI_849;
        syscomp = 'ANI_849';
    case 850
        ANI_850;
        syscomp = 'ANI_850';
    case 851
        ANI_851;
        syscomp = 'ANI_851';
    case 852
        ANI_852;
        syscomp = 'ANI_852';
end
```

D.9 COSMO-FILES (Matlab File)

D.9.1 ANIONS

[BF4] (Computation ID = 70)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.21
%   total number of segments         =    298
%   number of charge corr segments   =    202
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% F             1.56355676332522    1.56355676332522   -1.56355676332522   3.2503
0.2434    77.45     0.00314    5.7070
% F            -1.56355676332522    1.56355676332522    1.56355676332522   3.2503
0.2434    77.45     0.00314    5.7070
% F             1.56355676332522   -1.56355676332522    1.56355676332522   3.2503
0.2433    77.45     0.00314    5.7070
% F            -1.56355676332522   -1.56355676332522   -1.56355676332522   3.2503
0.2433    77.45     0.00314    5.7070
% B             0.00000000000000    0.00000000000000    0.00000000000000   3.8692
0.0253    15.82     0.00160    6.3259
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                  =       -424.794941
%   Total energy + OC corr.       =       -424.797657
%   Dielectric energy             =         -0.097554      -2.655      -61.22
%   Diel. energy + OC corr.       =         -0.100269      -2.728      -62.92
%
%   Surface area of cavity [au]
acosmo =           325.613;
%   Total Volume of cavity [au]
vcosmo =           495.525;
%
%
% $screening_charge
%   cosmo           =    0.98506
%   corrected total =    0.99883
%
%
% $segment information
```

```
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1     3.48878     3.36275    -3.46650      0.00314895    1.34967722
0.00233311   -0.18272746
    2    1     1.67972     0.87551    -4.73810      0.00337511    1.10428136
0.00305638   -0.19987932
    3    1     4.22923     0.28105    -2.91043      0.00363413    1.10428136
0.00329095   -0.19824424
    4    1     4.42131     2.61710    -0.42863      0.00321361    0.98158343
0.00327390   -0.19833578
    5    1     1.91005     4.71698    -0.85603      0.00371930    1.10428136
0.00336807   -0.19883756
    6    1    -0.01219     3.64074    -3.50442      0.00362922    1.10428136
0.00328650   -0.19906512
    7    1     2.90213     2.71062    -4.29434      0.00364283    1.47237514
0.00247412   -0.18510460
    8    1     2.37583     1.76202    -4.70450      0.00356567    1.22697929
0.00290606   -0.19128188
    9    1     4.04096     2.31006    -3.53078      0.00365942    1.47237514
0.00248538   -0.18520914
   10    1     4.27155     1.19610    -3.32324      0.00359530    1.22697929
0.00293020   -0.19128181
   11    1     4.16499     3.29170    -2.46404      0.00363451    1.47237514
0.00246846   -0.18499861
   12    1     4.37762     3.17131    -1.31666      0.00389563    1.34967722
0.00288634   -0.19087870
   13    1     3.17048     4.17073    -2.65224      0.00335403    1.34967722
0.00248506   -0.18463372
   14    1     2.55577     4.64808    -1.82042      0.00347765    1.22697929
0.00283432   -0.19022978
   15    1     2.38821     3.89570    -3.67206      0.00416393    1.71777100
0.00242403   -0.18468977
   16    1     1.17980     3.94655    -3.74043      0.00420724    1.47237514
0.00285745   -0.19070056
   17    1     2.67258     0.50051    -4.42793      0.00386146    1.22697929
0.00314713   -0.19751546
   18    1     3.54565     0.25203    -3.78074      0.00388739    1.22697929
0.00316826   -0.19704182
   19    1     4.69876     0.89031    -2.09457      0.00477815    1.47237514
0.00324520   -0.19744836
   20    1     4.78304     1.83402    -1.20787      0.00372260    1.22697929
0.00303396   -0.19698715
   21    1     3.75994     3.55291    -0.22822      0.00460637    1.47237514
0.00312853   -0.19711125
   22    1     2.89277     4.34297    -0.52778      0.00382403    1.22697929
0.00311662   -0.19654789
   23    1     1.23605     4.79361    -1.71909      0.00338756    1.10428136
0.00306766   -0.19749871
   24    1     0.55367     4.38914    -2.81292      0.00350415    1.10428136
0.00317324   -0.19670849
   25    1     0.41522     3.01036    -4.23802      0.00468603    1.47237514
0.00318263   -0.19680016
   26    1     1.10427     2.00854    -4.75036      0.00426144    1.34967722
0.00315738   -0.19664585
   27    1     1.96771    -0.03472    -4.36477      0.00256156    0.61348964
0.00417540   -0.20488858
```

```
   28    1     3.00532    -0.85010    -3.19457      0.00202382    0.61348964
0.00329886   -0.20628332
   29    1     3.63025    -0.60209    -2.82981      0.00334199    0.98158343
0.00340469   -0.20447015
   30    1     4.20224    -0.27233    -2.04472      0.00302913    1.10428136
0.00274308   -0.20590472
   31    1     4.46077     1.79956    -0.10918      0.00350311    0.98158343
0.00356884   -0.20472249
   32    1     3.83254     2.58688     0.52672      0.00394364    1.10428136
0.00357123   -0.20475103
   33    1     3.13350     3.14267     0.80423      0.00249297    0.73618757
0.00338632   -0.20589795
   34    1     1.97215     4.36246     0.03767      0.00329618    0.98158343
0.00335803   -0.20471393
   35    1     0.88604     4.67391    -0.90676      0.00289259    0.73618757
0.00392915   -0.20542982
   36    1    -0.63883     3.72167    -2.59150      0.00482319    1.47237514
0.00327579   -0.20523216
   37    1    -0.74002     2.76736    -3.51522      0.00397606    1.22697929
0.00324053   -0.20550101
   38    1     0.75926     1.02169    -4.66583      0.00426166    1.10428136
0.00385922   -0.20517772
   39    1     3.41781     1.47426    -4.23161      0.00407122    1.47237514
0.00276507   -0.18938882
   40    1     4.65896     2.18131    -2.33922      0.00465619    1.71777100
0.00271060   -0.18921025
   41    1     3.57293     4.11632    -1.46070      0.00404069    1.47237514
0.00274434   -0.18922101
   42    1     1.74144     4.60866    -2.68625      0.00442253    1.59507307
0.00277262   -0.18998291
   43    1     1.67344     2.94581    -4.50329      0.00408403    1.47237514
0.00277377   -0.18952615
   44    1     2.60173    -0.53596    -3.81719      0.00377847    1.10428136
0.00342166   -0.20467815
   45    1     4.67652     0.82686    -0.98784      0.00383145    0.98158343
0.00390333   -0.20513381
   46    1     2.77337     3.80302     0.45780      0.00345681    0.98158343
0.00352167   -0.20371763
   47    1     0.11148     4.44841    -1.92926      0.00432237    1.22697929
0.00352277   -0.20368065
   48    1    -0.14051     2.00479    -4.29597      0.00352136    1.22697929
0.00286995   -0.20500277
   49    2    -3.48875     3.36273     3.46655      0.00314904    1.34967722
0.00233318   -0.18272481
   50    2    -1.67970     0.87545     4.73810      0.00337432    1.10428136
0.00305567   -0.19986590
   51    2    -4.22922     0.28105     2.91041      0.00363322    1.10428136
0.00329012   -0.19824026
   52    2    -4.42128     2.61714     0.42866      0.00321267    0.98158343
0.00327294   -0.19832903
   53    2    -1.91001     4.71700     0.85611      0.00371962    1.10428136
0.00336836   -0.19883746
   54    2     0.01223     3.64069     3.50448      0.00362888    1.10428136
0.00328619   -0.19906453
   55    2    -2.90211     2.71057     4.29438      0.00364286    1.47237514
0.00247414   -0.18509968
```

```
   56    2    -2.37581     1.76197     4.70452      0.00356571    1.22697929
0.00290609   -0.19127419
   57    2    -4.04093     2.31004     3.53081      0.00365969    1.47237514
0.00248557   -0.18520625
   58    2    -4.27154     1.19609     3.32324      0.00359519    1.22697929
0.00293011   -0.19127808
   59    2    -4.16495     3.29171     2.46409      0.00363462    1.47237514
0.00246854   -0.18499712
   60    2    -4.37759     3.17134     1.31671      0.00389588    1.34967722
0.00288652   -0.19087708
   61    2    -3.17044     4.17072     2.65230      0.00335416    1.34967722
0.00248516   -0.18463214
   62    2    -2.55573     4.64809     1.82050      0.00347773    1.22697929
0.00283439   -0.19022886
   63    2    -2.38818     3.89567     3.67212      0.00416382    1.71777100
0.00242397   -0.18468592
   64    2    -1.17976     3.94650     3.74049      0.00420700    1.47237514
0.00285729   -0.19069567
   65    2    -2.67257     0.50046     4.42793      0.00386292    1.22697929
0.00314832   -0.19750828
   66    2    -3.54564     0.25200     3.78073      0.00388762    1.22697929
0.00316845   -0.19703956
   67    2    -4.69875     0.89033     2.09457      0.00477774    1.47237514
0.00324492   -0.19744012
   68    2    -4.78302     1.83405     1.20789      0.00372193    1.22697929
0.00303341   -0.19697941
   69    2    -3.75991     3.55296     0.22827      0.00460683    1.47237514
0.00312884   -0.19710664
   70    2    -2.89273     4.34300     0.52785      0.00382401    1.22697929
0.00311661   -0.19654670
   71    2    -1.23601     4.79361     1.71917      0.00338776    1.10428136
0.00306784   -0.19749735
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  235    4     0.64548    -1.46121    -3.96386      0.00723024    2.08803516
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  236    1    -0.64549     1.46123    -3.96385      0.00688567    2.08803516
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  237    1     0.77560     0.04015    -4.34026      0.00775431    2.08803516
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  238    1     1.86555    -1.04980    -3.65752      0.00317317    1.04060935
0.00304934   -0.20868043
  239    5     2.55679     2.35696     1.65864      0.00135793    0.82334525
0.00164928   -0.20663160
  240    1     2.65618     2.87070     1.17970      0.00240151    0.76665534
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  241    5    -1.65861     2.55678    -2.35700      0.00131953    0.82339864
0.00160254   -0.20664384
  242    1    -1.17966     2.65615    -2.87074      0.00232700    0.76670506
0.00303507   -0.20925677
  243    5     2.35700    -1.65859    -2.55680      0.00126038    0.82345480
0.00153060   -0.20671291
  244    1     2.87076    -1.17964    -2.65615      0.00229755    0.76675735
0.00299645   -0.20932668
  245    2    -1.93431    -1.36212     3.18964      0.00059096    0.16178096
0.00365287   -0.20975356
  246    3    -1.36215    -1.93429     3.18964      0.00076267    0.16178096
0.00471424   -0.20976014
  247    5    -1.72400    -1.72398     3.01901      0.00054046    0.16178096
0.00334071   -0.20877406
  248    2     1.36213     1.93428     3.18967      0.00073951    0.16178096
0.00457104   -0.20972954
  249    3     1.93429     1.36211     3.18967      0.00060174    0.16178096
0.00371950   -0.20973805
  250    5     1.72398     1.72397     3.01903      0.00055471    0.16178096
0.00342878   -0.20872953
  251    3     1.86559     1.04985     3.65746      0.00318604    1.04064736
0.00306160   -0.20866456
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  252    3     0.77560    -0.04013     4.34026      0.00764703    2.08811341
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  253    3    -0.64555    -1.46126     3.96381      0.00693058    2.08811341
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  254    2     0.64552     1.46125     3.96383      0.00688953    2.08811341
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  255    2    -0.77563     0.04012     4.34025      0.00775567    2.08811341
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  257    2    -3.18970     1.93426    -1.36209      0.00060132    0.16177855
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  258    4    -3.18971     1.36209    -1.93426      0.00073896    0.16177855
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  259    5    -3.01908     1.72394    -1.72394      0.00055355    0.16177855
0.00342164   -0.20874471
  260    2    -3.18967    -1.36210     1.93429      0.00077046    0.16177855
0.00476243   -0.20973000
  261    4    -3.18967    -1.93428     1.36212      0.00059602    0.16177855
0.00368418   -0.20972495
  262    5    -3.01904    -1.72396     1.72397      0.00056208    0.16177855
0.00347438   -0.20870622
  263    4    -3.65745    -1.86558     1.04985      0.00317709    1.04063289
0.00305304   -0.20866380
  264    4    -4.34025    -0.77562    -0.04010      0.00775572    2.08808324
0.00371428   -0.21249716
  265    4    -3.96384     0.64549    -1.46122      0.00688811    2.08808324
0.00329877   -0.21186030
  266    2    -3.96381    -0.64551     1.46126      0.00693382    2.08808324
0.00332066   -0.21191920
  267    2    -4.34025     0.77560     0.04015      0.00764696    2.08808324
0.00366219   -0.21253013
  268    2    -3.65748     1.86556    -1.04982      0.00318489    1.04063289
0.00306054   -0.20867021
  269    5    -2.35700    -1.65865     2.55675      0.00130537    0.82331823
0.00158550   -0.20661635
  270    2    -2.87072    -1.17969     2.65615      0.00231048    0.76663018
0.00301381   -0.20929338
  271    5    -2.55678     2.35698    -1.65862      0.00132719    0.82339767
0.00161185   -0.20665844
  272    2    -2.65615     2.87073    -1.17967      0.00239578    0.76670414
0.00312478   -0.20931606
  273    5     1.65866     2.55676     2.35698      0.00131524    0.82333443
0.00159746   -0.20661509
  274    2     1.17971     2.65615     2.87071      0.00233400    0.76664526
0.00304443   -0.20924676
  275    3    -1.36215    -3.18965     1.93429      0.00059505    0.16177593
0.00367822   -0.20972557
  276    4    -1.93431    -3.18965     1.36212      0.00076872    0.16177593
0.00475174   -0.20972749
  277    5    -1.72399    -3.01902     1.72397      0.00055887    0.16177593
0.00345462   -0.20870614
  278    3     1.93424    -3.18975    -1.36206      0.00073954    0.16177593
0.00457139   -0.20973289
  279    4     1.36208    -3.18975    -1.93423      0.00060145    0.16177593
0.00371778   -0.20974125
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  280    5     1.72393    -3.01912    -1.72392      0.00055466    0.16177593
0.00342856   -0.20873459
  281    4     1.04980    -3.65752    -1.86553      0.00318596    1.04062559
0.00306158   -0.20866690
  282    4    -0.04017    -4.34027    -0.77556      0.00764721    2.08806883
0.00366234   -0.21252720
  283    4    -1.46129    -3.96381     0.64554      0.00693261    2.08806883
0.00332011   -0.21191799
  284    3     1.46120    -3.96387    -0.64546      0.00688916    2.08806883
0.00329930   -0.21185741
  285    3     0.04007    -4.34025     0.77566      0.00775586    2.08806883
0.00371437   -0.21249389
  286    3    -1.04989    -3.65744     1.86560      0.00317628    1.04062559
0.00305228   -0.20866003
  287    5    -1.65867    -2.55676     2.35697      0.00132669    0.82330505
0.00161142   -0.20658432
  288    3    -1.17973    -2.65615     2.87070      0.00229711    0.76661791
0.00299642   -0.20930134
  289    5     2.35700     1.65863     2.55676      0.00134293    0.82333472
0.00163109   -0.20663594
  290    3     2.87073     1.17968     2.65615      0.00239417    0.76664554
0.00312292   -0.20931507
  291    5     2.55681    -2.35699    -1.65858      0.00129508    0.82344064
0.00157276   -0.20665140
  292    3     2.65616    -2.87074    -1.17963      0.00233270    0.76674416
0.00304235   -0.20924817
  293    5    -2.55678    -2.35697     1.65864      0.00132732    0.82332263
0.00161215   -0.20653014
  294    4    -2.65617    -2.87070     1.17970      0.00230668    0.76663427
0.00300885   -0.20929514
  295    5     1.65861    -2.55680    -2.35699      0.00136007    0.82344838
0.00165168   -0.20662804
  296    4     1.17965    -2.65616    -2.87074      0.00239696    0.76675137
0.00312612   -0.20931458
  297    5    -2.35697     1.65861    -2.55680      0.00128402    0.82340570
0.00155940   -0.20667731
  298    4    -2.87072     1.17966    -2.65616      0.00233145    0.76671162
0.00304085   -0.20925083];
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[EtSO4] (Computation ID = 71)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.38
%   total number of segments         =    580
%   number of charge corr segments   =    287
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% S             3.34959947046329   -1.72885297259872   -0.07856788061644   4.0818
0.0579    34.00     0.00170    6.5385
% O            -0.54637671846446   -1.46543386052232   -0.83111204138626   3.2503
0.2194    44.27     0.00496    5.7070
% O             5.45200736387592   -2.26311298650331    2.77544158951322   3.2503
0.2640    68.65     0.00384    5.7070
% O             3.94836939390913   -4.00422315375165   -1.65098198881673   3.2503
0.2831    74.69     0.00379    5.7070
% O             4.31757613980175    0.81335614099148   -0.96973821519503   3.2503
0.2557    67.73     0.00377    5.7070
% C            -1.46480058684167    0.89631718145962   -0.02722295977428   3.7795
0.0337    29.84     0.00113    6.2361
% C            -4.26592271143034    1.11581020313455   -0.73884221947503   3.7795
0.0540    58.86     0.00092    6.2361
% H            -0.39530748613840    2.47788431420660   -0.90269022772338   2.4566  -
0.0038    20.59    -0.00018    4.9133
% H            -1.28740645670125    1.13522891730114    2.05859370328902   2.4566  -
0.0113    26.80    -0.00042    4.9133
% H            -5.36552612806333   -0.41178609636959    0.15382312090475   2.4566  -
0.0186    25.10    -0.00074    4.9133
% H            -4.50480300222913    0.95329542501327   -2.80149025443080   2.4566  -
0.0189    25.08    -0.00075    4.9133
% H            -5.05511186862902    2.95087784433539   -0.12332488548480   2.4566  -
0.0260    24.65    -0.00106    4.9133
% H             5.81770259044746   -0.46936095669651    3.13611225919581   2.4566  -
0.0914    28.97    -0.00315    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -779.180819
%   Total energy + OC corr.      =       -779.186446
%   Dielectric energy            =         -0.102473      -2.788      -64.30
%   Diel. energy + OC corr.      =         -0.108101      -2.942      -67.84
%
%   Surface area of cavity [au]
acosmo =           529.220;
```

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%   Total Volume of cavity [au]
vcosmo =           906.441;
%
%
% $screening_charge
%   cosmo           =    0.96196
%   corrected total =    0.99784
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1     2.35795    -5.16838     1.88288      0.00033989    0.96751531
0.00035130   -0.19521410
    2    1     2.41298    -1.14132    -4.00778      0.00075413    0.58050918
0.00129908   -0.21642758
    3    1     6.96309    -1.61374    -1.97349      0.00073616    0.38700612
0.00190219   -0.21512204
    4    1     1.24261    -2.38669     3.35493      0.00107074    0.77401224
0.00138337   -0.18280756
    5    1     1.49858    -5.18977     1.04249      0.00094813    0.96751531
0.00097996   -0.20247577
    6    1     3.13350    -1.22209    -4.12303      0.00058848    0.58050918
0.00101372   -0.21769169
    7    1     7.23249    -1.95863    -1.31617      0.00068437    0.58050918
0.00117891   -0.21171843
    8    1     1.65342    -4.55012     2.33483     -0.00060010    1.54802449   -
0.00038766   -0.18802524
    9    1     0.84595    -3.48639     2.62398      0.00111437    1.16101837
0.00095982   -0.18976763
   10    1     2.09476    -0.79157    -3.84792      0.00063484    0.38700612
0.00164038   -0.21675762
   11    1     1.51864    -3.63495     3.03196      0.00118407    0.96751531
0.00122383   -0.18800026
   12    1     0.96284    -4.68061     1.42193     -0.00019614    0.96751531   -
0.00020273   -0.19846086
   13    1     7.36167    -1.88675    -0.81318      0.00096439    0.77401224
0.00124597   -0.21000284
   14    2    -2.57702    -3.71819    -1.99991      0.00441229    0.98158343
0.00449508   -0.20601538
   15    2    -1.20947    -4.01279     1.07569      0.00766980    1.22697929
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   16    2    -0.54349    -2.08719    -4.02140      0.00395735    0.73618757
0.00537546   -0.22290940
   17    2    -0.96198    -4.44018    -2.07315      0.00316986    0.61348964
0.00516694   -0.22404979
   18    2    -1.76946    -4.24354    -1.99330      0.00533028    1.22697929
0.00434423   -0.21556440
   19    2    -0.91965    -4.56221     0.08279      0.00470050    0.85888550
0.00547279   -0.22316893
   20    2    -0.49491    -2.96580    -3.71395      0.00450644    0.85888550
0.00524685   -0.22668903
   21    2    -2.39503    -4.13883    -0.82908      0.00512175    0.98158343
0.00521785   -0.21082558
   22    2    -1.83900    -4.28682     0.13507      0.00607361    1.10428136
0.00550005   -0.21645394
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   27    2    -2.12512    -3.44820     1.20379      0.00761215    1.10428136
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   28    2    -1.24690    -3.16146     1.85169      0.00625854    1.22697929
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   29    2     0.13164    -0.34829    -3.80716      0.00228805    0.36809379
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   30    2    -0.47843    -0.86127    -4.02406      0.00568791    0.98158343
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   37    3     5.09217    -5.48595     2.99570      0.00246528    0.73618757
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   38    3     4.48177    -4.08469     5.28646      0.00616410    1.22697929
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   41    3     6.66548    -1.71234     5.74003      0.00233780    0.98158343
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   42    3     8.58094    -1.38430     2.73108      0.00408427    1.22697929
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   43    3     3.43230    -0.89652     4.92438      0.00478186    1.10428136
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   44    3     4.41542    -5.27178     3.43736      0.00374338    1.10428136
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   45    3     4.60576    -4.89764     4.48069      0.00427735    0.98158343
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   46    3     5.93326    -5.47631     2.86706      0.00421600    1.22697929
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   47    3     6.72771    -5.14523     3.56955      0.00483781    1.22697929
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   49    3     6.61240    -4.62782     4.67973      0.00555883    1.34967722
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   50    3     7.82089    -4.48384     2.92152      0.00666923    1.47237514
0.00452957   -0.20510184
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   54    3     7.63263    -1.62631     5.10009      0.00143500    0.85888550
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   55    3     8.36667    -1.55551     4.02787      0.00223351    0.98158343
0.00227541   -0.15422657
   56    3     8.32227    -1.14002     1.74357      0.00362700    0.98158343
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   57    3     4.44260    -1.10197     5.63858      0.00364844    0.98158343
0.00371690   -0.16127424
   58    3     5.52040    -1.36568     5.89868      0.00300727    1.10428136
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   59    3     5.30303    -3.42507     5.80734      0.00623426    1.34967722
0.00461908   -0.18850514
   60    3     5.94251    -2.48362     5.98098      0.00497309    1.34967722
0.00368465   -0.17130025
   61    3     7.24389    -2.65737     5.45842      0.00510325    1.71777100
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   62    3     7.51282    -3.67873     4.85240      0.00519979    1.34967722
0.00385262   -0.18342269
   63    3     8.26388    -3.49821     3.83964      0.00608209    1.47237514
0.00413080   -0.18867460
   64    3     8.65865    -2.48238     3.25905      0.00659344    1.59507307
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   65    3     8.59133    -2.28645     1.93365      0.00667695    1.34967722
0.00494707   -0.19881664
   66    3     8.19283    -2.87684     1.13968      0.00622307    1.10428136
0.00563540   -0.21645746
   67    3     3.03703    -1.86644     4.91444      0.00481978    0.85888550
0.00561167   -0.19241863
   68    3     3.72537    -1.92930     5.50895      0.00645569    1.22697929
0.00526145   -0.18627387
   69    3     4.02406    -3.07195     5.58107      0.00734419    1.34967722
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   70    3     5.57660    -5.22066     4.11787      0.00572625    1.47237514
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   71    3     6.96468    -5.10792     2.34707      0.00572362    1.34967722
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  554   11    -3.37812     2.53808    -4.20642     -0.00057367    0.55923837   -
0.00102581   -0.10556200
```

```
  555    7    -4.86478    -1.44536    -3.38390     -0.00006376    0.54295233   -
0.00011743   -0.12655204
  556    7    -6.24929    -0.76508    -3.27717     -0.00000274    0.54295233   -
0.00000506   -0.10574544
  557    7    -6.92509     0.62538    -3.30846     -0.00001906    0.54295233   -
0.00003510   -0.09392555
  558    7    -6.60228     2.12955    -3.46435     -0.00009548    0.54295233   -
0.00017585   -0.09022057
  559    7    -5.41935     3.10221    -3.67797      0.00001969    0.54295233
0.00003626   -0.09378378
  560    7    -3.88371     3.12613    -3.85769     -0.00010634    0.54295233   -
0.00019586   -0.10259864
  561    7    -2.79441     2.50124    -3.93460     -0.00006343    0.30369508   -
0.00020885   -0.11624124
  562   12    -3.72971     4.96511    -0.59370     -0.00013366    0.24915167   -
0.00053646   -0.08796095
  563   12    -4.51101     4.90318    -1.41083     -0.00046179    0.55404171   -
0.00083349   -0.08417358
  564   12    -5.75639     4.50332    -1.81547     -0.00042542    0.55404171   -
0.00076784   -0.08060410
  565   12    -6.88700     3.86925    -1.37472     -0.00046503    0.55404171   -
0.00083935   -0.07710960
  566   12    -7.43079     3.26572    -0.27262     -0.00055594    0.55404171   -
0.00100343   -0.07567223
  567   12    -7.16070     2.94472     1.03068     -0.00045502    0.55404171   -
0.00082128   -0.07723427
  568   12    -6.18951     3.04027     1.99102     -0.00043527    0.55404171   -
0.00078562   -0.07989534
  569   12    -4.92272     3.51249     2.20742     -0.00062509    0.55404171   -
0.00112825   -0.08244893
  570    7    -3.71152     4.78186    -1.16530     -0.00037760    0.54194011   -
0.00069676   -0.09235678
  571    7    -4.94365     4.54638    -2.04306     -0.00014629    0.54194011   -
0.00026993   -0.08866808
  572    7    -6.34738     3.93554    -2.02172     -0.00002727    0.54194011   -
0.00005032   -0.08424762
  573    7    -7.33661     3.20437    -1.11021     -0.00017085    0.54194011   -
0.00031525   -0.08092088
  574    7    -7.49832     2.65816     0.31090     -0.00004056    0.54194011   -
0.00007485   -0.08139407
  575    7    -6.76497     2.52496     1.64826     -0.00004588    0.54194011   -
0.00008466   -0.08423457
  576    7    -5.44278     2.86040     2.34347     -0.00016155    0.54194011   -
0.00029810   -0.08714233
  577    7    -4.30487     3.36349     2.30257      0.00001156    0.30200203
0.00003826   -0.09050037
  578   13     3.62315     1.19885     3.76839     -0.00053806    0.88704675   -
0.00060657   -0.12475028
  579   13     3.44356     0.67099     4.16656      0.00006147    0.88704675
0.00006929   -0.13089762
  580    9     1.03747     1.47973     3.56398      0.00052671    1.76462677
0.00029848   -0.13170389];
```

[TF_2N] (Computation ID = 72)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.21
%   total number of segments         =    585
%   number of charge corr segments   =    411
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% S            -2.73903414385911   -0.28380581186837    0.96816804921008   4.0818
0.0000     0.00     0.00000    6.5385
% S             2.64055896767402    1.40179690834613    0.66611145883206   4.0818
0.0000     0.00     0.00000    6.5385
% N             0.05465566331351   -0.04577390983394   -0.77063111904768   3.4582
0.0493    31.22     0.00158    5.9148
% C            -5.11438104721446   -0.29921324785314   -1.52617906941304   3.7795
0.0000     0.00     0.00000    6.2361
% C             5.21951226374820   -0.73460918573127   -0.13161653735625   3.7795
0.0000     0.00     0.00000    6.2361
% O            -3.38956176858350    2.22010884272696    2.83048533893264   3.2503
0.2104    69.13     0.00304    5.7070
% O             3.35931490469745    4.22826033208055   -0.63390854195366   3.2503
0.2277    79.18     0.00288    5.7070
% O             2.51662151409236    1.51838389043995    3.84686573291615   3.2503
0.2052    67.91     0.00302    5.7070
% O            -3.03829738076342   -3.06176424242443    2.51454054843941   3.2503
0.2276    80.34     0.00283    5.7070
% F            -7.57992972990917   -0.50493807269097   -0.45110232878784   3.2503
0.0075    71.33     0.00010    5.7070
% F            -4.76811588072517   -2.39729401992860   -3.22259586643056   3.2503
0.0132    72.06     0.00018    5.7070
% F            -5.03086817459247    1.96770198681176   -3.01264790999449   3.2503
0.0172    70.39     0.00024    5.7070
% F             5.53702070245438   -0.94686705645513   -2.81797052045941   3.2503
0.0117    71.84     0.00016    5.7070
% F             4.78445257806757   -3.23326261791721    0.83479871175637   3.2503
0.0184    71.38     0.00026    5.7070
% F             7.54805153159983    0.17127620429770    0.90568205335623   3.2503
0.0109    71.60     0.00015    5.7070
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =      -1827.741788
%   Total energy + OC corr.      =      -1827.745432
%   Dielectric energy            =         -0.081373      -2.214      -51.06
```

```
%   Diel. energy + OC corr.      =         -0.085017      -2.313      -53.35
%
%   Surface area of cavity [au]
acosmo =           756.375;
%   Total Volume of cavity [au]
vcosmo =          1541.846;
%
%
% $screening_charge
%   cosmo           =    0.97766
%   corrected total =    0.99906
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    3     0.05787     0.88950    -4.09994      0.00206180    0.83336214
0.00247407   -0.14829878
    2    3     0.47456    -2.38732    -3.28060      0.00180668    0.69446845
0.00260152   -0.14177980
    3    3     0.81858     1.00182    -3.97656      0.00157388    0.69446845
0.00226630   -0.14724183
    4    3     0.02358    -0.13454    -4.22754      0.00236877    0.83336214
0.00284243   -0.14295093
    5    3     0.40644    -1.15748    -4.02630      0.00253523    0.83336214
0.00304217   -0.14072157
    6    3     0.62990    -2.90438    -2.62981      0.00092431    0.27778738
0.00332741   -0.14409677
    7    3     0.19295     1.73288    -3.73311      0.00222522    0.55557476
0.00400525   -0.15543881
    8    3     0.26395    -3.00505    -2.54770      0.00084953    0.27778738
0.00305819   -0.14459615
    9    3     0.69717     0.12585    -4.16426      0.00128859    0.55557476
0.00231938   -0.14341552
   10    3     0.28174    -3.34718    -1.77475      0.00196325    0.55557476
0.00353373   -0.14882159
   11    6    -4.02006     4.83084     4.66113      0.00159450    1.34967722
0.00118140   -0.16403531
   12    6    -5.49848     4.51845     1.91684      0.00300234    0.85888550
0.00349562   -0.16724676
   13    6    -2.43553     5.19766     1.94235      0.00345069    0.85888550
0.00401764   -0.18857451
   14    6    -3.46980     1.79802     6.05229      0.00385865    1.22697929
0.00314484   -0.19026859
   15    6    -6.30123     2.31426     4.27197      0.00356277    0.85888550
0.00414813   -0.17340802
   16    6    -4.81596     4.98609     3.76827      0.00233349    1.47237514
0.00158485   -0.16243972
   17    6    -5.19207     4.92027     2.67316      0.00297361    1.22697929
0.00242352   -0.16576313
   18    6    -3.43085     5.33506     3.75791      0.00238598    1.47237514
0.00162050   -0.16990744
   19    6    -2.83400     5.42208     2.77133      0.00329952    1.22697929
0.00268914   -0.18043127
   20    6    -2.89313     4.68199     4.89383      0.00185462    1.34967722
0.00137412   -0.17361878
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   21    6    -2.03251     4.19733     5.02451      0.00272673    0.98158343
0.00277789   -0.18727167
   22    6    -3.85293     4.00802     5.50506      0.00188423    1.34967722
0.00139606   -0.16841515
   23    6    -3.77308     2.97096     5.96956      0.00269141    1.22697929
0.00219352   -0.17730103
   24    6    -5.01369     4.12868     4.90032      0.00245878    1.71777100
0.00143138   -0.16272442
   25    6    -5.84722     3.27889     4.67534      0.00356881    1.47237514
0.00242384   -0.16727956
   26    6    -4.46348     5.01725     1.57056      0.00469676    1.22697929
0.00382791   -0.17294188
   27    6    -3.42933     5.30261     1.80028      0.00288880    0.85888550
0.00336342   -0.17977279
   28    6    -1.81946     5.06284     2.96641      0.00393958    0.73618757
0.00535132   -0.19314176
   29    6    -2.20635     2.84351     5.79293      0.00173581    0.49079171
0.00353676   -0.19422637
   30    6    -2.62345     2.23319     5.98921      0.00371405    1.10428136
0.00336332   -0.19382610
   31    6    -4.54284     1.81281     5.84191      0.00438510    1.34967722
0.00324900   -0.18389910
   32    6    -5.61996     2.09780     5.19161      0.00397560    1.22697929
0.00324015   -0.17725525
   33    6    -6.38540     3.21692     3.60243      0.00446016    1.34967722
0.00330461   -0.16740491
   34    6    -6.11039     3.97800     2.56313      0.00507989    1.34967722
0.00376379   -0.16536105
   35    6    -2.76229     4.91685     1.12788      0.00313666    0.49079171
0.00639103   -0.18758483
   36    6    -2.72741     1.06217     5.79450      0.00440401    0.98158343
0.00448663   -0.20187351
   37    6    -4.02322     0.81532     5.69223      0.00529597    1.10428136
0.00479585   -0.19543352
   38    6    -5.55721     0.68069     4.70025      0.00313533    0.49079171
0.00638832   -0.18707406
   39    6    -6.02013     1.43704     4.57159      0.00445156    0.98158343
0.00453508   -0.18025317
   40    6    -4.10889     5.38724     2.70170      0.00347119    1.47237514
0.00235754   -0.17009133
   41    6    -2.14213     4.99792     3.96733      0.00411106    1.71777100
0.00239325   -0.18426184
   42    6    -2.76297     3.53650     5.73551      0.00253375    1.34967722
0.00187730   -0.18130842
   43    6    -4.90660     2.95263     5.61017      0.00355714    1.59507307
0.00223008   -0.17165768
   44    6    -5.77767     4.24831     3.69531      0.00290971    1.34967722
0.00215586   -0.16322079
   45    6    -3.44466     4.95143     1.06935      0.00183028    0.49079171
0.00372924   -0.18162071
   46    6    -5.14748     1.04705     5.29994      0.00396950    0.98158343
0.00404397   -0.18781864
   47    7     4.10115     7.06251    -2.04153      0.00153985    1.34967722
0.00114090   -0.14816595
   48    7     1.49583     5.27292    -3.08354      0.00410296    1.10428136
0.00371550   -0.17170577
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   49    7     4.52383     4.38120    -3.66459      0.00328947    0.85888550
0.00382993   -0.15935330
   50    7     6.43378     5.23149    -0.95927      0.00330829    0.85888550
0.00385184   -0.15836183
   51    7     4.60926     6.55312     1.26278      0.00374153    1.22697929
0.00304938   -0.17294195
   52    7     1.38919     6.70020     0.12296      0.00328135    0.98158343
0.00334292   -0.18075584
   53    7     3.04227     6.82219    -2.56669      0.00223680    1.47237514
0.00151918   -0.15305321
   54    7     2.15646     6.11567    -2.99091      0.00331202    1.34967722
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   55    7     4.32326     6.30978    -2.93667      0.00238519    1.47237514
0.00161996   -0.14984334
   56    7     4.43591     5.30858    -3.50417      0.00313259    1.22697929
0.00255309   -0.15535219
   57    7     5.20830     6.62157    -1.82471      0.00219974    1.47237514
0.00149401   -0.14888358
   58    7     6.02138     5.98000    -1.27381      0.00310354    1.34967722
0.00229947   -0.15420715
   59    7     4.45762     7.27349    -0.92548      0.00179475    1.34967722
0.00132976   -0.15139371
   60    7     4.53120     7.14200     0.20366      0.00257007    1.22697929
0.00209463   -0.16045094
   61    7     3.19643     7.41181    -1.26886      0.00219860    1.71777100
0.00127991   -0.15385652
   62    7     2.20238     7.26545    -0.59212      0.00321226    1.47237514
0.00218168   -0.16580065
   63    7     2.40238     4.98399    -3.64683      0.00401319    1.22697929
0.00327079   -0.16667473
   64    7     3.41371     4.73710    -3.84368      0.00327475    0.98158343
0.00333619   -0.16252180
   65    7     5.31257     4.71978    -3.18494      0.00284000    0.85888550
0.00330661   -0.15601332
   66    7     6.17063     5.03318    -2.05278      0.00366504    1.10428136
0.00331893   -0.15516745
   67    7     6.21030     5.64391     0.02374      0.00460136    1.34967722
0.00340923   -0.16272455
   68    7     5.46756     6.31681     0.69198      0.00356415    1.22697929
0.00290481   -0.16652796
   69    7     3.57651     6.90632     1.19519      0.00398931    1.34967722
0.00295575   -0.17478154
   70    7     2.32248     6.99135     0.72811      0.00437826    1.47237514
0.00297360   -0.17733162
   71    7     1.25031     6.67087    -1.02183      0.00390115    1.34967722
0.00289043   -0.17394339
   72    7     1.19852     6.14584    -2.12337      0.00384440    1.22697929
0.00313323   -0.17183926
   73    7     1.71845     4.20365    -3.43953      0.00481980    0.98158343
0.00491023   -0.17371223
   74    7     3.63524     3.95499    -3.86094      0.00293609    0.73618757
0.00398824   -0.16378316
   75    7     5.10401     5.58986     1.74660      0.00580718    1.22697929
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   76    7     3.77743     6.11293     1.98104      0.00497236    1.10428136
0.00450280   -0.18566564
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   77    7     1.94682     6.08915     1.62590      0.00350437    0.61348964
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   78    7     1.38935     6.24240     0.98698      0.00449036    0.98158343
0.00457460   -0.18983385
   79    7     0.77260     6.12866    -0.12195      0.00355050    0.73618757
0.00482282   -0.18624425
   80    7     0.90964     5.36291    -2.44396      0.00261719    0.61348964
0.00426607   -0.17685457
   81    7     3.27728     5.84373    -3.45315      0.00340492    1.47237514
0.00231254   -0.15678740
   82    7     5.44561     5.72504    -2.62680      0.00339897    1.59507307
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   83    7     5.45889     6.70041    -0.42178      0.00294488    1.47237514
0.00200009   -0.15587510
   84    7     3.37408     7.39524     0.09738      0.00314749    1.59507307
0.00197326   -0.16286385
   85    7     2.02303     6.90164    -1.91142      0.00279814    1.34967722
0.00207319   -0.16179015
   86    7     2.54918     3.73868    -3.74333      0.00503969    1.22697929
0.00410740   -0.16854420
   87    7     5.94478     4.45137    -2.59099      0.00262689    0.61348964
0.00428188   -0.15592917
   88    7     5.80105     5.50275     1.09187      0.00387097    0.85888550
0.00450697   -0.17163110
   89    7     2.66206     6.44501     1.63867      0.00362324    0.98158343
0.00369122   -0.18685539
   90    7     0.58619     5.84454    -1.14584      0.00445801    0.98158343
0.00454165   -0.18253807
   91    8     2.35352     1.54949     7.09296      0.00158626    1.34967722
0.00117529   -0.16641445
   92    8     4.23480    -0.55501     5.66718      0.00368150    0.98158343
0.00375057   -0.17017761
   93    8     2.39928     4.41924     5.30834      0.00323376    0.98158343
0.00329443   -0.18892252
   94    8     5.15613     2.57266     5.42358      0.00356986    0.85888550
0.00415638   -0.17410431
   95    8     3.19236     0.70043     6.91916      0.00235249    1.47237514
0.00159775   -0.16517833
   96    8     3.69512    -0.17959     6.35539      0.00298392    1.22697929
0.00243192   -0.16895734
   97    8     1.77479     0.53667     6.85530      0.00224189    1.47237514
0.00152263   -0.17364558
   98    8     1.37629    -0.40472     6.20612      0.00314337    0.98158343
0.00320235   -0.18549779
   99    8     1.35123     1.82122     6.86596      0.00155232    1.10428136
0.00140573   -0.17529531
  100    8     0.78410     2.30091     6.48330      0.00192624    0.98158343
0.00196238   -0.18482317
  101    8     2.27491     2.71418     6.85956      0.00183750    1.34967722
0.00136143   -0.16965304
  102    8     2.37038     3.68265     6.26745      0.00265371    1.22697929
0.00216280   -0.17739135
  103    8     3.44244     2.11219     6.90545      0.00245862    1.71777100
0.00143128   -0.16422570
  104    8     4.46070     2.37843     6.30562      0.00356269    1.47237514
0.00241969   -0.16830967
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  105    8     3.16790    -1.06008     5.71557      0.00365067    0.98158343
0.00371916   -0.17662670
  106    8     1.85028    -0.98419     5.81101      0.00240895    0.73618757
0.00327220   -0.18578077
  107    8     0.78175     0.28072     6.30108      0.00239524    0.73618757
0.00325357   -0.18885177
  108    8     0.89906     3.65397     5.68737      0.00141843    0.49079171
0.00289009   -0.19385621
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[Cl] (Computation ID = 73)

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%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.36
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%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
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% $end
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%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                  =       -460.427467
%   Total energy + OC corr.       =       -460.435960
%   Dielectric energy             =         -0.120087      -3.268      -75.36
%   Diel. energy + OC corr.       =         -0.128580      -3.499      -80.69
%
%   Surface area of cavity [au]
acosmo =           188.589;
%   Total Volume of cavity [au]
vcosmo =           243.527;
%
%
% $screening_charge
%   cosmo           =    0.96538
%   corrected total =    0.99893
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1    -3.87226     0.01876    -0.11184      0.01026071    1.91725882
0.00535176   -0.25756143
    2    1    -1.73530    -2.62123    -2.26388      0.00939679    1.74296257
0.00539127   -0.25766584
    3    1    -1.73699     1.26518    -3.22329      0.00936117    1.74296257
0.00537084   -0.25765324
    4    1    -1.80860     3.42408     0.10995      0.00943990    1.74296257
0.00541601   -0.25767760
    5    1    -1.86774     0.92729     3.26482      0.00937827    1.74296257
0.00538065   -0.25766150
```

```
    6    1    -1.68056    -2.96373     1.84371      0.00857516    1.56866631
0.00546653   -0.25780031
    7    1     1.86800    -0.92726    -3.26469      0.00937850    1.74296257
0.00538078   -0.25766038
    8    1     1.68031     2.96374    -1.84401      0.00857458    1.56866631
0.00546616   -0.25779654
    9    1     1.73494     2.62116     2.26429      0.00939649    1.74296257
0.00539110   -0.25766341
   10    1     1.73745    -1.26534     3.22298      0.00936186    1.74296257
0.00537123   -0.25765317
   11    1     1.80871    -3.42401    -0.11007      0.00944067    1.74296257
0.00541645   -0.25767803
   12    1     3.87300     0.03720     0.07750      0.01108687    2.09155508
0.00530078   -0.25742953
   13    1    -3.58947    -1.17333    -0.86383      0.01103386    2.09155508
0.00527543   -0.25741267
   14    1    -2.81228    -2.03348    -1.72142      0.01024172    1.91725882
0.00534185   -0.25752365
   15    1    -3.57207     0.42995    -1.43622      0.01104472    2.09155508
0.00528062   -0.25741414
   16    1    -2.82139     0.79922    -2.53147      0.00944704    1.74296257
0.00542011   -0.25765301
   17    1    -3.59888     1.43349    -0.02222      0.01103034    2.09155508
0.00527375   -0.25740425
   18    1    -2.87282     2.57968     0.31546      0.01019970    1.91725882
0.00531994   -0.25752210
   19    1    -3.64892     0.43673     1.22552      0.01030512    1.91725882
0.00537493   -0.25753670
   20    1    -2.98202     0.61970     2.39391      0.00933610    1.74296257
0.00535645   -0.25764860
   21    1    -3.62312    -1.08202     0.84228      0.01275756    2.44014759
0.00522819   -0.25719841
   22    1    -2.87362    -2.15806     1.44648      0.01108120    2.09155508
0.00529807   -0.25743518
   23    1     3.59917    -1.43283     0.02192      0.01104823    2.09155508
0.00528230   -0.25740725
   24    1     2.87291    -2.57958    -0.31554      0.01019863    1.91725882
0.00531938   -0.25752220
   25    1     3.57247    -0.43001     1.43530      0.01106271    2.09155508
0.00528923   -0.25741718
   26    1     2.82235    -0.79870     2.53059      0.00944627    1.74296257
0.00541966   -0.25765296
   27    1     3.58935     1.17401     0.86362      0.01103967    2.09155508
0.00527821   -0.25741041
   28    1     2.81168     2.03417     1.72167      0.01024035    1.91725882
0.00534114   -0.25752085
   29    1     3.60354     1.11454    -0.88312      0.01193380    2.26585133
0.00526681   -0.25730266
   30    1     2.87359     2.15810    -1.44660      0.01106317    2.09155508
0.00528945   -0.25742637
   31    1     3.64879    -0.43678    -1.22602      0.01030614    1.91725882
0.00537546   -0.25753438
   32    1     2.98164    -0.62014    -2.39432      0.00933438    1.74296257
0.00535547   -0.25764557
   33    1    -1.93787    -1.50605    -2.99730      0.01012534    1.91725882
0.00528115   -0.25751443
```

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   34    1    -1.99970    -0.12826    -3.31543      0.01010722    1.91725882
0.00527170   -0.25749521
   35    1    -2.01478     2.23938    -2.43582      0.01192791    2.26585133
0.00526421   -0.25730983
   36    1    -2.04271     3.08799    -1.13977      0.01107909    2.09155508
0.00529706   -0.25743831
   37    1    -1.96141     2.97642     1.51698      0.01108923    2.09155508
0.00530191   -0.25742928
   38    1    -2.03417     2.04308     2.58754      0.01098713    2.09155508
0.00525309   -0.25739156
   39    1    -1.99609    -0.36929     3.29948      0.01019879    1.91725882
0.00531946   -0.25753814
   40    1    -1.97601    -1.87220     2.75636      0.01104755    2.09155508
0.00528198   -0.25743023
   41    1    -1.98947    -3.25812     0.65868      0.01184802    2.26585133
0.00522895   -0.25729439
   42    1    -2.01896    -3.17103    -0.93573      0.01197719    2.26585133
0.00528596   -0.25733132
   43    1     1.99609     0.36930    -3.29951      0.01019982    1.91725882
0.00532000   -0.25753593
   44    1     1.97649     1.87226    -2.75602      0.01104822    2.09155508
0.00528230   -0.25742659
   45    1     1.98977     3.25801    -0.65859      0.01184874    2.26585133
0.00522927   -0.25729002
   46    1     2.01929     3.17094     0.93552      0.01197773    2.26585133
0.00528619   -0.25732784
   47    1     1.93838     1.50598     2.99703      0.01012494    1.91725882
0.00528095   -0.25751297
   48    1     1.99936     0.12805     3.31566      0.01010812    1.91725882
0.00527217   -0.25749462
   49    1     2.01461    -2.23936     2.43598      0.01192785    2.26585133
0.00526418   -0.25730984
   50    1     2.04248    -3.08808     1.13992      0.01107927    2.09155508
0.00529715   -0.25743855
   51    1     1.96141    -2.97656    -1.51670      0.01108950    2.09155508
0.00530204   -0.25742940
   52    1     2.03391    -2.04308    -2.58775      0.01098643    2.09155508
0.00525276   -0.25739107
   53    1    -0.66765    -2.24256    -3.08748      0.01017746    1.91725882
0.00530834   -0.25752984
   54    1     0.63741    -1.74690    -3.39845      0.01109221    2.09155508
0.00530333   -0.25740938
   55    1     0.58498    -0.18153    -3.82522      0.01273700    2.44014759
0.00521976   -0.25715907
   56    1    -0.66209     0.55918    -3.77576      0.01018278    1.91725882
0.00531111   -0.25750900
   57    1    -0.51313     1.98805    -3.28509      0.01104383    2.09155508
0.00528020   -0.25742171
   58    1     0.60928     2.72626    -2.68399      0.01195529    2.26585133
0.00527629   -0.25732623
   59    1     0.51269     3.59624    -1.34600      0.01024199    1.91725882
0.00534199   -0.25755438
   60    1    -0.61418     3.78199    -0.57172      0.01104278    2.09155508
0.00527970   -0.25741133
   61    1    -0.67349     3.67483     1.02445      0.01196921    2.26585133
0.00528243   -0.25733625
```

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   62    1     0.58513     3.37101     1.81698      0.01189087    2.26585133
0.00524786   -0.25729760
   63    1     0.66753     2.24252     3.08755      0.01017698    1.91725882
0.00530809   -0.25752858
   64    1    -0.63769     1.74685     3.39842      0.01109168    2.09155508
0.00530308   -0.25740911
   65    1    -0.58495     0.18167     3.82520      0.01273783    2.44014759
0.00522011   -0.25715957
   66    1     0.66258    -0.55918     3.77567      0.01018340    1.91725882
0.00531144   -0.25750900
   67    1     0.51261    -1.98788     3.28525      0.01104361    2.09155508
0.00528009   -0.25742224
   68    1    -0.60910    -2.72620     2.68405      0.01195596    2.26585133
0.00527659   -0.25732805
   69    1    -0.51276    -3.59620     1.34599      0.01024279    1.91725882
0.00534241   -0.25755665
   70    1     0.61439    -3.78194     0.57166      0.01104338    2.09155508
0.00527998   -0.25741264
   71    1     0.67316    -3.67486    -1.02450      0.01196945    2.26585133
0.00528254   -0.25733743
   72    1    -0.58470    -3.37091    -1.81725      0.01189102    2.26585133
0.00524792   -0.25729964
   73    1    -3.05038    -0.68585    -2.28737      0.01099251    2.09155508
0.00525566   -0.25739148
   74    1    -3.08880     1.95501    -1.28241      0.01272215    2.44014759
0.00521368   -0.25718667
   75    1    -3.06851     1.78010     1.55654      0.01098867    2.09155508
0.00525383   -0.25739350
   76    1    -2.99032    -0.79630     2.33048      0.01186212    2.26585133
0.00523517   -0.25728779
   77    1    -3.04960    -2.38493    -0.13877      0.01110303    2.09155508
0.00530851   -0.25742909
   78    1     3.08863    -1.95517     1.28263      0.01272120    2.44014759
0.00521329   -0.25718749
   79    1     3.05022     0.68546     2.28775      0.01099307    2.09155508
0.00525593   -0.25739095
   80    1     3.04987     2.38465     0.13896      0.01108978    2.09155508
0.00530217   -0.25742208
   81    1     2.98980     0.79701    -2.33096      0.01184552    2.26585133
0.00522784   -0.25728087
   82    1     3.06889    -1.77975    -1.55624      0.01098930    2.09155508
0.00525413   -0.25739292
   83    1    -0.79405    -0.90665    -3.68169      0.01022083    1.91725882
0.00533096   -0.25754279
   84    1    -0.78840     3.17241    -2.07888      0.01190568    2.26585133
0.00525440   -0.25732130
   85    1    -0.68256     2.87233     2.50824      0.01105510    2.09155508
0.00528559   -0.25740698
   86    1    -0.82140    -1.35319     3.53575      0.01108417    2.09155508
0.00529949   -0.25742130
   87    1    -0.76717    -3.78944    -0.24259      0.01192261    2.26585133
0.00526187   -0.25731297
   88    1     0.82123     1.35327    -3.53578      0.01108371    2.09155508
0.00529927   -0.25741997
   89    1     0.76670     3.78957     0.24268      0.01192202    2.26585133
0.00526161   -0.25731036
```

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   90    1     0.79397     0.90659     3.68173      0.01022091    1.91725882
0.00533100   -0.25754217
   91    1     0.78874    -3.17234     2.07881      0.01190603    2.26585133
0.00525455   -0.25732213
   92    1     0.68292    -2.87235    -2.50810      0.01105492    2.09155508
0.00528550   -0.25740773];
```

[PF_6] (Computation ID = 74)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.21
%   total number of segments         =    348
%   number of charge corr segments   =    252
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% P             0.00000000000000    0.00000000000000    0.00000000000000   4.0062
0.0000     0.00     0.00000    6.4629
% F             3.14706298320938    0.00000000000000    0.00000000000000   3.2503
0.1665    68.33     0.00244    5.7070
% F            -3.14706298320938    0.00000000000000    0.00000000000000   3.2503
0.1664    68.33     0.00244    5.7070
% F             0.00000000000000    3.14706298320938    0.00000000000000   3.2503
0.1665    68.33     0.00244    5.7070
% F             0.00000000000000   -3.14706298320938    0.00000000000000   3.2503
0.1665    68.33     0.00244    5.7070
% F             0.00000000000000    0.00000000000000    3.14706298320938   3.2503
0.1665    68.33     0.00244    5.7070
% F             0.00000000000000    0.00000000000000   -3.14706298320938   3.2503
0.1665    68.33     0.00244    5.7070
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                  =       -941.063720
%   Total energy + OC corr.       =       -941.066147
%   Dielectric energy             =         -0.088698      -2.414      -55.66
%   Diel. energy + OC corr.       =         -0.091125      -2.480      -57.18
%
%   Surface area of cavity [au]
acosmo =           409.970;
%   Total Volume of cavity [au]
vcosmo =           701.945;
%
%
% $screening_charge
%   cosmo           =    0.98534
%   corrected total =    0.99889
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]           charge       area [au]
charge/area    potential [au]
```

```
%
data = [1    2     6.39600    -0.09381     0.01576      0.00174973    1.34967722
0.00129640   -0.16085936
    2    2     4.84425    -1.76823    -2.13481      0.00209145    0.85888550
0.00243508   -0.17992890
    3    2     4.69850    -2.67958     0.98869      0.00253518    0.98158343
0.00258274   -0.18190500
    4    2     4.74483     0.02333     2.83043      0.00259557    0.98158343
0.00264427   -0.18171081
    5    2     4.76161     2.70806     0.79020      0.00322494    1.10428136
0.00292040   -0.18119102
    6    2     4.55712     1.54693    -2.48663      0.00267674    1.10428136
0.00242396   -0.18304210
    7    2     6.15874    -0.72476    -0.98443      0.00218374    1.47237514
0.00148314   -0.16385043
    8    2     5.54401    -1.45187    -1.64660      0.00245229    1.22697929
0.00199864   -0.17153284
    9    2     6.14413    -1.20500     0.36077      0.00219808    1.47237514
0.00149288   -0.16404324
   10    2     5.51429    -2.12394     0.67059      0.00247682    1.22697929
0.00201863   -0.17200359
   11    2     6.16662    -0.01862     1.20276      0.00217737    1.47237514
0.00147881   -0.16376382
   12    2     5.55743     0.26470     2.16443      0.00263260    1.34967722
0.00195054   -0.17145530
   13    2     6.20861     1.02827     0.36645      0.00197896    1.34967722
0.00146625   -0.16326014
   14    2     5.64906     2.00857     0.51996      0.00234225    1.22697929
0.00190895   -0.17034171
   15    2     6.18697     0.70671    -0.90782      0.00244305    1.71777100
0.00142222   -0.16341348
   16    2     5.55813     1.21365    -1.81065      0.00287458    1.47237514
0.00195234   -0.17129678
   17    2     4.82058    -2.45154    -1.32432      0.00257548    1.10428136
0.00233227   -0.18012161
   18    2     4.91484    -2.72687    -0.06066      0.00278936    1.10428136
0.00252595   -0.17949066
   19    2     5.00680    -1.99588     1.76705      0.00262955    1.10428136
0.00238123   -0.17795667
   20    2     4.86095    -0.95627     2.59092      0.00371222    1.47237514
0.00252124   -0.17969199
   21    2     4.95939     1.25514     2.38849      0.00236074    0.98158343
0.00240503   -0.17870648
   22    2     4.97894     2.11927     1.64854      0.00257498    1.10428136
0.00233182   -0.17829216
   23    2     4.87009     2.73891    -0.30706      0.00289350    1.22697929
0.00235823   -0.17996325
   24    2     5.04556     2.19510    -1.46352      0.00277246    1.22697929
0.00225958   -0.17747795
   25    2     4.97084     0.62329    -2.61723      0.00297096    1.10428136
0.00269040   -0.17871879
   26    2     4.99601    -0.78800    -2.55440      0.00230877    0.98158343
0.00235209   -0.17836252
   27    2     4.13042    -2.30383    -2.07120      0.00198089    0.61348964
0.00322889   -0.18784017
   28    2     4.10786    -2.43653     1.92479      0.00239921    0.73618757
0.00325896   -0.18808588
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   29    2     4.42792     0.99293     2.81749      0.00163554    0.61348964
0.00266596   -0.18551514
   30    2     4.23288     2.54245     1.70931      0.00134575    0.61348964
0.00219360   -0.18698375
   31    2     4.16373     2.17237    -2.19359      0.00197322    0.61348964
0.00321638   -0.18749898
   32    2     4.39394    -1.47671    -2.61326      0.00211804    0.61348964
0.00345245   -0.18542839
   33    2     5.70643    -1.91914    -0.57542      0.00271225    1.47237514
0.00184209   -0.16952545
   34    2     5.73865    -1.07595     1.64032      0.00305463    1.71777100
0.00177825   -0.16900694
   35    2     5.72162     1.30600     1.49357      0.00268674    1.47237514
0.00182477   -0.16930078
   36    2     5.70742     1.91435    -0.58692      0.00252226    1.34967722
0.00186879   -0.16955732
   37    2     5.70578    -0.11642    -2.00099      0.00266296    1.47237514
0.00180862   -0.16954998
   38    2     4.47663    -2.85150    -0.81591      0.00166639    0.49079171
0.00339532   -0.18494183
   39    2     4.32306    -1.80668     2.43261      0.00185176    0.73618757
0.00251533   -0.18576352
   40    2     4.20496     1.94769     2.37742      0.00237082    0.73618757
0.00322040   -0.18707563
   41    2     4.34558     2.69820    -1.35940      0.00240497    0.73618757
0.00326678   -0.18607842
   42    2     4.66323    -0.09009    -2.87361      0.00167436    0.61348964
0.00272924   -0.18289885
   43    3    -6.39602    -0.09386    -0.01570      0.00174976    1.34967722
0.00129643   -0.16086003
   44    3    -4.84423    -1.76826     2.13487      0.00209173    0.85888550
0.00243540   -0.17992964
   45    3    -4.69851    -2.67961    -0.98863      0.00251901    0.98158343
0.00256627   -0.18186541
   46    3    -4.74488     0.02328    -2.83038      0.00258630    0.98158343
0.00263483   -0.18168462
   47    3    -4.76166     2.70802    -0.79017      0.00323156    1.10428136
0.00292639   -0.18120803
   48    3    -4.55712     1.54692     2.48667      0.00269444    1.10428136
0.00243999   -0.18308295
   49    3    -6.15874    -0.72480     0.98449      0.00218375    1.47237514
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   50    3    -5.54400    -1.45190     1.64666      0.00245219    1.22697929
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  214    7     0.02329    -2.83039    -4.74483      0.00258195    0.98158343
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  215    7     2.70802    -0.79016    -4.76162      0.00322597    1.10428136
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  216    7     1.54691     2.48667    -4.55710      0.00267634    1.10428136
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  217    7    -0.72480     0.98448    -6.15871      0.00218351    1.47237514
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  221    7    -0.01866    -1.20271    -6.16661      0.00217708    1.47237514
0.00147862   -0.16376600
  222    7     0.26466    -2.16439    -5.55743      0.00263265    1.34967722
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  223    7     1.02823    -0.36640    -6.20860      0.00197866    1.34967722
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  224    7     2.00853    -0.51992    -5.64906      0.00234215    1.22697929
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  225    7     0.70667     0.90787    -6.18695      0.00244259    1.71777100
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  227    7    -2.45157     1.32437    -4.82053      0.00257795    1.10428136
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  231    7     1.25510    -2.38845    -4.95939      0.00236096    0.98158343
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  232    7     2.11923    -1.64850    -4.97895      0.00257445    1.10428136
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  236    7    -0.78803     2.55445    -4.99597      0.00230726    0.98158343
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  242    7    -1.47674     2.61330    -4.39389      0.00211921    0.61348964
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  261    4     2.90990     3.73106    -1.40628      0.00566381    1.95239840
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  267    6     2.40605    -2.40605     2.98580      0.00192791    0.60812473
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  269    5     2.40607    -2.98577    -2.40606      0.00192693    0.60812330
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  270    7     2.40607    -2.40602    -2.98580      0.00194586    0.60812330
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  348    5    -1.94909    -3.54171    -2.72058      0.00279191    0.97416959
0.00286594   -0.19131399];
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[$MOEtSO_4$] (Computation ID = 75)

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% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.30
%   total number of segments         =    685
%   number of charge corr segments   =    331
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% S             6.03843003753744    0.77188118774521    0.40836402879729   4.0818
0.0520    28.17     0.00185    6.5385
% O             7.82028759821076   -1.35146141671299   -0.03077571542694   3.2503
0.2872    75.18     0.00382    5.7070
% O             5.79839450235637    1.65147639233901    3.07953877546308   3.2503
0.2763    71.01     0.00389    5.7070
% O             3.18427837118605   -0.77635229676447   -0.17349414785116   3.2503
0.1367    37.43     0.00365    5.7070
% O             6.08244000343297    2.84388558555818   -1.50656219878545   3.2503
0.2771    71.57     0.00387    5.7070
% C             1.05473351173081    0.86015414063633    0.12169453906120   3.7795
0.0088    26.23     0.00034    6.2361
% C            -1.27265831819718   -0.79270095430950   -0.20988840596913   3.7795
0.0028    26.28     0.00011    6.2361
% O            -3.51789986441533    0.75215280604824   -0.06187437890702   3.2503
0.1410    38.22     0.00369    5.7070
% C            -5.73817094378358   -0.72920201800950   -0.33189767371970   3.7795
0.0143    66.19     0.00022    6.2361
% H             1.05916139137524    1.74057641032489    2.01266096689967   2.4566  -
0.0224    21.16    -0.00106    4.9133
% H             1.07758402523218    2.37911073512919   -1.30927958935075   2.4566  -
0.0227    22.30    -0.00102    4.9133
% H            -1.32581622527612   -2.26301674100739    1.27756341156103   2.4566  -
0.0301    25.20    -0.00120    4.9133
% H            -1.20377286686625   -1.76090526572615   -2.06418046914503   2.4566  -
0.0293    25.12    -0.00117    4.9133
% H            -5.92311218464323   -2.14017595974675    1.20951343838558   2.4566  -
0.0274    24.72    -0.00111    4.9133
% H            -5.77056682676971   -1.75151709877828   -2.16356902164994   2.4566  -
0.0272    24.47    -0.00111    4.9133
% H            -7.36331221111044    0.56609449327405   -0.25781355936275   2.4566  -
0.0387    24.13    -0.00160    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                  =       -893.201338
```

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%   Total energy + OC corr.      =       -893.206201
%   Dielectric energy            =         -0.105582      -2.873      -66.25
%   Diel. energy + OC corr.      =         -0.110445      -3.005      -69.31
%
%   Surface area of cavity [au]
acosmo =           607.382;
%   Total Volume of cavity [au]
vcosmo =          1069.036;
%
%
% $screening_charge
%   cosmo           =    0.96364
%   corrected total =    0.99831
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1     5.70821    -0.90350    -3.29909      0.00090875    0.58050918
0.00156544   -0.21160410
    2    1     9.64274     1.67619     2.09729      0.00040880    0.96751531
0.00042252   -0.20247139
    3    1     6.49716    -0.40889    -3.47191      0.00064579    0.38700612
0.00166868   -0.21736659
    4    1     9.82919     1.96318    -0.52560      0.00081224    0.96751531
0.00083951   -0.20701842
    5    1     9.93662     1.84424     0.97006      0.00020768    1.35452143
0.00015332   -0.19775266
    6    1     9.53030     0.89443     2.51860      0.00106553    0.58050918
0.00183550   -0.21276461
    7    1     5.75625    -2.29988     3.08151      0.00108479    0.96751531
0.00112122   -0.21362517
    8    1     5.62286    -0.35456    -3.49286      0.00068832    0.38700612
0.00177858   -0.21160214
    9    1     8.87574     3.59711     1.20152      0.00050122    1.74152755
0.00028780   -0.20219316
   10    1     9.38748     2.72187     1.69006      0.00017523    1.35452143
0.00012937   -0.19720919
   11    1     9.64816     2.67735     0.38794      0.00015986    1.35452143
0.00011802   -0.19727836
   12    1     5.01137    -2.22057     2.98740      0.00073406    0.77401224
0.00094839   -0.20905163
   13    2     9.95627    -3.74893    -0.53503      0.00338441    1.34967722
0.00250757   -0.19451675
   14    2    10.11006    -1.88033     2.21465      0.00444819    1.10428136
0.00402813   -0.21448184
   15    2    10.89312    -0.55470    -0.72902      0.00505437    1.22697929
0.00411936   -0.21298022
   16    2     8.85257    -1.89316    -3.06483      0.00455716    1.10428136
0.00412681   -0.21537437
   17    2     6.75283    -3.99602    -1.59005      0.00522069    1.22697929
0.00425492   -0.21263233
   18    2     7.35567    -4.01353     1.77536      0.00414748    0.98158343
0.00422529   -0.21498879
   19    2    10.23070    -3.43934     0.59793      0.00400724    1.47237514
0.00272161   -0.19749319
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   20    2    10.32694    -2.69254     1.54493      0.00454890    1.34967722
0.00337036   -0.20531684
   21    2    10.67318    -2.80082    -0.60077      0.00399009    1.47237514
0.00270997   -0.19742538
   22    2    10.99992    -1.69166    -0.61286      0.00410509    1.22697929
0.00334569   -0.20441359
   23    2     9.82497    -3.32301    -1.66135      0.00403150    1.47237514
0.00273809   -0.19757565
   24    2     9.27853    -2.79194    -2.55329      0.00459645    1.34967722
0.00340559   -0.20534974
   25    2     8.99442    -4.19675    -1.07492      0.00364313    1.34967722
0.00269926   -0.19666724
   26    2     7.89349    -4.32686    -1.33696      0.00387786    1.22697929
0.00316050   -0.20298227
   27    2     9.15078    -4.30589     0.22557      0.00457626    1.71777100
0.00266407   -0.19695833
   28    2     8.30613    -4.36272     1.09210      0.00493850    1.47237514
0.00335410   -0.20465009
   29    2    10.72941    -1.43039     1.41679      0.00470761    1.22697929
0.00383675   -0.21129348
   30    2    11.02145    -0.96808     0.38187      0.00518297    1.34967722
0.00384016   -0.21044127
   31    2    10.60560    -0.96108    -1.65995      0.00568901    1.47237514
0.00386383   -0.21171911
   32    2     9.80267    -1.42071    -2.60564      0.00570010    1.47237514
0.00387136   -0.21323364
   33    2     8.03684    -2.73863    -2.96222      0.00594336    1.47237514
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   34    2     7.45147    -3.60358    -2.34517      0.00412374    1.10428136
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   35    2     6.73259    -4.36798    -0.56188      0.00518913    1.34967722
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   36    2     7.14500    -4.42517     0.78215      0.00418129    1.10428136
0.00378643   -0.21101863
   37    2     8.36800    -3.68141     2.16832      0.00530405    1.34967722
0.00392986   -0.21248442
   38    2     9.33853    -2.82646     2.43580      0.00618169    1.59507307
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   39    2    10.14313    -0.77675     2.16896      0.00508871    1.22697929
0.00414734   -0.21964524
   40    2    10.70422     0.13491     0.16510      0.00450165    1.22697929
0.00366889   -0.21661942
   41    2    10.39580     0.28357    -1.15241      0.00508990    1.10428136
0.00460924   -0.22013616
   42    2     8.86968    -0.86773    -3.06876      0.00549457    1.10428136
0.00497570   -0.22325545
   43    2     7.75077    -1.61816    -3.26938      0.00608048    1.34967722
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   44    2     6.66357    -3.35823    -2.31099      0.00210580    0.49079171
0.00429063   -0.21727930
   45    2     6.43728    -3.77475     1.63643      0.00485948    1.10428136
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   46    2     7.36335    -3.30141     2.52922      0.00588325    1.22697929
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   52    2     9.41269    -3.71902     1.52600      0.00476345    1.47237514
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   53    2    10.57781    -0.23984     1.28265      0.00506916    1.10428136
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   63    3     6.53856     1.94865     6.23050      0.00410949    1.47237514
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  128    5     6.46592     6.06581    -1.69838      0.00416657    1.22697929
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  145    5     5.96337     5.55729     0.27888      0.00427303    0.85888550
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  146    5     5.71488     3.39643    -4.68844      0.00479313    1.47237514
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  147    5     7.84976     4.09571    -3.93025      0.00545839    1.71777100
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  639    9    -6.15075    -4.40039     0.17648     -0.00050591    0.55629013   -
0.00090943   -0.05739110
  640    9    -4.89529    -4.34670     0.37627     -0.00012248    0.31102331   -
0.00039378   -0.06452928
  641   15    -4.85187    -4.02947    -2.19133     -0.00023811    0.25344431   -
0.00093948   -0.06125215
  642   15    -5.98757    -4.14068    -2.10919     -0.00068952    0.56422550   -
0.00122206   -0.05445101
  643   15    -7.24663    -3.63205    -2.37081     -0.00082695    0.56422550   -
0.00146564   -0.04832430
  644   15    -7.88623    -2.55664    -2.95972     -0.00080674    0.56422550   -
0.00142982   -0.04726644
  645   15    -7.63476    -1.37112    -3.62583     -0.00065625    0.56422550   -
0.00116310   -0.05205465
  646   15    -6.59902    -0.57890    -4.08628     -0.00073106    0.56422550   -
0.00129568   -0.05942143
  647   15    -5.21881    -0.51640    -4.14556     -0.00091966    0.56422550   -
0.00162995   -0.06722166
  648    9    -5.22413    -4.15018    -1.72918     -0.00038642    0.55083758   -
0.00070152   -0.06150353
  649    9    -6.76337    -4.01151    -1.77937     -0.00045405    0.55083758   -
0.00082430   -0.05340065
  650    9    -7.88614    -3.07479    -2.28233     -0.00067094    0.55083758   -
0.00121804   -0.04831520
  651    9    -8.11567    -1.73780    -3.02448     -0.00042718    0.55083758   -
0.00077552   -0.05122553
  652    9    -7.35447    -0.56827    -3.69067     -0.00031650    0.55083758   -
0.00057458   -0.05905881
  653    9    -5.92580    -0.06283    -3.99802     -0.00047960    0.55083758   -
0.00087067   -0.06896859
  654    9    -4.68079    -0.22756    -3.92809     -0.00026314    0.30720522   -
0.00085656   -0.07800681
  655   16    -6.96534     2.93048    -0.79817     -0.00038937    0.23924144   -
0.00162751   -0.07233113
  656   16    -7.36674     2.47939    -1.71602     -0.00095891    0.52936641   -
0.00181143   -0.06413365
  657   16    -8.12488     1.56226    -2.31079     -0.00088264    0.52936641   -
0.00166734   -0.05509036
  658   16    -8.93486     0.53280    -2.07884     -0.00091791    0.52936641   -
0.00173399   -0.04717594
  659   16    -9.47684    -0.20250    -1.11175     -0.00103534    0.52936641   -
0.00195581   -0.04158911
  660   16    -9.53683    -0.35328     0.20859     -0.00106210    0.52936641   -
0.00200636   -0.04153503
  661   16    -9.09112     0.13997     1.36085     -0.00090634    0.52936641   -
0.00171212   -0.04719489
  662   16    -8.31573     1.08251     1.89004     -0.00085410    0.52936641   -
0.00161343   -0.05521194
  663   16    -7.51681     2.10215     1.58720     -0.00095433    0.52936641   -
0.00180278   -0.06430517
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  664   16    -7.03950     2.74407     0.83410     -0.00037690    0.23924144   -
0.00157540   -0.07243812
  665    9    -6.70914     2.74735    -1.29584     -0.00077172    0.52264247   -
0.00147657   -0.07743372
  666    9    -7.39544     1.94635    -2.34518     -0.00059428    0.52264247   -
0.00113707   -0.06558709
  667    9    -8.31914     0.79970    -2.55890     -0.00052935    0.52264247   -
0.00101284   -0.05557909
  668    9    -9.11553    -0.23984    -1.85260     -0.00058032    0.52264247   -
0.00111036   -0.04733130
  669    9    -9.47012    -0.76179    -0.50518     -0.00083227    0.52264247   -
0.00159243   -0.04316236
  670    9    -9.24291    -0.56006     0.95133     -0.00064061    0.52264247   -
0.00122571   -0.04731298
  671    9    -8.52362     0.28570     1.94180     -0.00054323    0.52264247   -
0.00103939   -0.05580342
  672    9    -7.59625     1.44154     2.07513     -0.00054883    0.52264247   -
0.00105011   -0.06578821
  673    9    -6.82701     2.45105     1.29867     -0.00082687    0.52264247   -
0.00158209   -0.07737559
  674   14    -4.38739    -4.30049     1.34012     -0.00025982    0.89343629   -
0.00029081   -0.06472755
  675   14    -4.39092    -3.81507     2.45366     -0.00178340    1.78699825   -
0.00099799   -0.06192301
  676   14    -4.36911    -2.56517     3.23563     -0.00182766    1.78699825   -
0.00102275   -0.06782640
  677   12    -2.98026    -4.18372     1.80147     -0.00180341    1.78699825   -
0.00100919   -0.07118002
  678   12    -2.97416    -3.30087     2.98245     -0.00197555    1.78699825   -
0.00110551   -0.07263631
  679   12    -2.94925    -2.15118     3.37386     -0.00036276    0.89343629   -
0.00040603   -0.08228227
  680   15    -4.14123    -1.15456    -4.16684     -0.00033330    0.90126667   -
0.00036981   -0.07189299
  681   15    -4.14586    -2.38220    -4.07024     -0.00207103    1.80288216   -
0.00114874   -0.06251358
  682   15    -4.16886    -3.53667    -3.12301     -0.00167912    1.80288216   -
0.00093135   -0.06203565
  683   13    -2.74293    -1.63098    -4.13465     -0.00198512    1.80288216   -
0.00110108   -0.07568360
  684   13    -2.75585    -3.05212    -3.67557     -0.00197705    1.80288216   -
0.00109660   -0.07039282
  685   13    -2.77873    -3.79696    -2.69518     -0.00026527    0.90126667   -
0.00029433   -0.07395028];
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[$C_2H_5OC_2H_4OSO_3$] (Computation ID = 76)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.33
%   total number of segments         =    797
%   number of charge corr segments   =    367
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% S             7.42627572729177    0.56351947577303    0.15503651380478   4.0818
0.0519    28.20     0.00184    6.5385
% O             9.21387402459925   -1.58063143217079   -0.12731472118910   3.2503
0.2867    75.18     0.00381    5.7070
% O             7.17526683974124    1.62558655751744    2.75767704875505   3.2503
0.2773    71.92     0.00386    5.7070
% O             4.56944756624051   -1.03588518626915   -0.32621241907160   3.2503
0.1372    37.37     0.00367    5.7070
% O             7.46698466479011    2.49673152671043   -1.89840745321195   3.2503
0.2773    71.73     0.00387    5.7070
% C             2.44804311969816    0.63350943422950   -0.27149520826007   3.7795
0.0063    22.61     0.00028    6.2361
% C             0.12832979314687   -1.02937901984752    0.06284269289884   3.7795
0.0043    26.20     0.00017    6.2361
% O            -2.13119208080606    0.49024487851406   -0.15265543263003   3.2503
0.1401    36.05     0.00389    5.7070
% C            -4.35808930341790   -0.99468386362141    0.16230379765887   3.7795
0.0067    32.01     0.00021    6.2361
% C            -6.65984559817329    0.68972909258369   -0.18520943278049   3.7795
0.0385    59.09     0.00065    6.2361
% H             2.61145453129177    1.98160505407209    1.31281849590068   2.4566  -
0.0212    21.54    -0.00098    4.9133
% H             2.30601848888237    1.72537616092868   -2.04822521819118   2.4566  -
0.0229    23.88    -0.00096    4.9133
% H             0.17852143681166   -1.96219934907852    1.93498360860889   2.4566  -
0.0274    26.51    -0.00103    4.9133
% H             0.11333452721695   -2.52991730795628   -1.39632758548987   2.4566  -
0.0284    24.77    -0.00115    4.9133
% H            -4.37508606143475   -2.56315293232002   -1.23225597350805   2.4566  -
0.0244    24.45    -0.00100    4.9133
% H            -4.37210305504713   -1.87119301506199    2.06967032705667   2.4566  -
0.0244    24.71    -0.00099    4.9133
% H            -8.41457193568170   -0.41327933273680    0.03647599245287   2.4566  -
0.0313    24.34    -0.00129    4.9133
% H            -6.65770890374102    1.55350282597818   -2.07848131326337   2.4566  -
0.0240    25.09    -0.00095    4.9133
```

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% H            -6.66895378140876    2.22051643275537    1.22477628045915   2.4566   -
0.0241    25.07    -0.00096    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -932.525610
%   Total energy + OC corr.      =       -932.530450
%   Dielectric energy            =         -0.105845      -2.880      -66.42
%   Diel. energy + OC corr.      =         -0.110685      -3.012      -69.46
%
%   Surface area of cavity [au]
acosmo =           680.705;
%   Total Volume of cavity [au]
vcosmo =          1213.712;
%
%
% $screening_charge
%   cosmo           =    0.96039
%   corrected total =    0.99827
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1     7.11461    -1.36807    -3.42727      0.00081637    0.58050918
0.00140630   -0.21202923
    2    1    11.02181     1.59233     1.79058      0.00039351    0.96751531
0.00040672   -0.20221010
    3    1     7.90323    -0.88492    -3.63121      0.00077377    0.38700612
0.00199938   -0.21821632
    4    1    11.21832     1.69544    -0.84521      0.00082161    0.96751531
0.00084920   -0.20669650
    5    1    11.31991     1.68175     0.65552      0.00018825    1.35452143
0.00013898   -0.19745616
    6    1    10.90928     0.84173     2.26515      0.00104026    0.58050918
0.00179198   -0.21246300
    7    1     7.13961    -2.31422     3.03557      0.00109893    0.96751531
0.00113583   -0.21395333
    8    1     7.02891    -0.83425    -3.65934      0.00076209    0.38700612
0.00196920   -0.21235373
    9    1    10.25447     3.44402     0.75952      0.00048901    1.74152755
0.00028080   -0.20178485
   10    1    10.76603     2.60634     1.31015      0.00016530    1.35452143
0.00012204   -0.19687716
   11    1    11.03209     2.47138     0.01536      0.00011694    1.35452143
0.00008633   -0.19687488
   12    1     6.39495    -2.24344     2.93323      0.00067205    0.77401224
0.00086827   -0.20946735
   13    2    11.35685    -4.00248    -0.45422      0.00337927    1.34967722
0.00250376   -0.19466493
   14    2    11.49767    -1.94365     2.15680      0.00446901    1.10428136
0.00404698   -0.21452654
   15    2    12.28711    -0.82767    -0.87091      0.00503612    1.22697929
0.00410449   -0.21287671
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   16    2    10.25704    -2.33307    -3.11230      0.00456378    1.10428136
0.00413280   -0.21559048
   17    2     8.15736    -4.33152    -1.49877      0.00517281    1.22697929
0.00421589   -0.21315598
   18    2     8.74951    -4.10939     1.86124      0.00413244    0.98158343
0.00420998   -0.21519740
   19    2    11.62697    -3.61283     0.65482      0.00400794    1.47237514
0.00272209   -0.19760251
   20    2    11.71852    -2.80066     1.54689      0.00454998    1.34967722
0.00337116   -0.20538109
   21    2    12.07183    -3.05962    -0.58472      0.00398322    1.47237514
0.00270530   -0.19749361
   22    2    12.39610    -1.95329    -0.67427      0.00409924    1.22697929
0.00334092   -0.20440551
   23    2    11.22819    -3.65763    -1.60824      0.00402332    1.47237514
0.00273254   -0.19773347
   24    2    10.68339    -3.19235    -2.53717      0.00458676    1.34967722
0.00339841   -0.20554242
   25    2    10.39774    -4.48975    -0.96397      0.00363922    1.34967722
0.00269636   -0.19691269
   26    2     9.29795    -4.64080    -1.21947      0.00387401    1.22697929
0.00315736   -0.20333970
   27    2    10.55020    -4.50622     0.34145      0.00457318    1.71777100
0.00266227   -0.19715346
   28    2     9.70293    -4.50369     1.20727      0.00492853    1.47237514
0.00334733   -0.20485035
   29    2    12.11854    -1.54975     1.33099      0.00470168    1.22697929
0.00383192   -0.21126427
   30    2    12.41283    -1.16110     0.26683      0.00517655    1.34967722
0.00383540   -0.21037672
   31    2    12.00348    -1.29960    -1.77162      0.00567252    1.47237514
0.00385263   -0.21168311
   32    2    11.20460    -1.82696    -2.68483      0.00567617    1.47237514
0.00385511   -0.21328285
   33    2     9.44290    -3.17118    -2.95259      0.00591838    1.47237514
0.00401961   -0.21352284
   34    2     8.85751    -3.99175    -2.27766      0.00409837    1.10428136
0.00371134   -0.21103971
   35    2     8.13468    -4.62985    -0.44693      0.00517013    1.34967722
0.00383064   -0.21184055
   36    2     8.54293    -4.59079     0.89901      0.00417924    1.10428136
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   37    2     9.75983    -3.74779     2.23277      0.00529787    1.34967722
0.00392529   -0.21263373
   38    2    10.72757    -2.87367     2.44202      0.00617441    1.59507307
0.00387093   -0.21338069
   39    2    11.52840    -0.84599     2.03324      0.00504834    1.22697929
0.00411444   -0.21955018
   40    2    12.09380    -0.07700    -0.02840      0.00446436    1.22697929
0.00363850   -0.21647163
   41    2    11.78925    -0.02268    -1.35404      0.00508049    1.10428136
0.00460072   -0.21996154
   42    2    10.27185    -1.31045    -3.18873      0.00549151    1.10428136
0.00497292   -0.22335372
   43    2     9.15528    -2.07596    -3.33913      0.00610592    1.34967722
0.00452399   -0.22245721
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   44    2     8.06895    -3.74655    -2.26330      0.00216274    0.49079171
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   45    2     7.83103    -3.88331     1.70299      0.00481333    1.10428136
0.00435879   -0.22019387
   46    2     8.75318    -3.34571     2.56284      0.00592760    1.22697929
0.00483105   -0.22134306
   47    2    10.74126    -1.66973     2.74041      0.00531573    1.10428136
0.00481375   -0.22263359
   48    2    12.28221    -2.45366     0.49537      0.00459348    1.47237514
0.00311978   -0.20227088
   49    2    11.79547    -2.59668    -1.82070      0.00532278    1.71777100
0.00309865   -0.20272400
   50    2     9.94558    -4.08428    -2.06661      0.00463116    1.47237514
0.00314537   -0.20296960
   51    2     9.26797    -4.82947    -0.04564      0.00498805    1.59507307
0.00312716   -0.20304656
   52    2    10.80665    -3.82817     1.59788      0.00476123    1.47237514
0.00323371   -0.20356342
   53    2    11.96468    -0.37205     1.11249      0.00508721    1.10428136
0.00460681   -0.21703811
   54    2    11.26172    -0.66515    -2.47951      0.00575051    1.34967722
0.00426065   -0.22127866
   55    2     8.27810    -3.03735    -2.87809      0.00557132    1.22697929
0.00454068   -0.22009102
   56    2     7.81862    -4.41354     0.64241      0.00336049    0.73618757
0.00456472   -0.21679185
   57    2     9.65685    -2.64102     2.91309      0.00558155    1.22697929
0.00454902   -0.22282625
   58    3     6.87290     2.76056     5.78837      0.00348460    1.34967722
0.00258180   -0.18904076
   59    3     9.28252     0.54132     4.98219      0.00495545    1.22697929
0.00403874   -0.21394283
   60    3     6.17278    -0.31726     5.16290      0.00456017    1.10428136
0.00412954   -0.20713661
   61    3     6.26778     4.72704     3.10710      0.00402181    0.98158343
0.00409727   -0.20709217
   62    3     9.43870     3.77874     3.65508      0.00421332    0.98158343
0.00429237   -0.21092658
   63    3     7.90550     2.14435     5.88215      0.00409549    1.47237514
0.00278155   -0.19378843
   64    3     8.63748     1.27806     5.63966      0.00424679    1.22697929
0.00346117   -0.20263137
   65    3     6.57921     1.61868     5.95289      0.00416838    1.47237514
0.00283106   -0.19174802
   66    3     6.34942     0.51434     5.69840      0.00431172    1.22697929
0.00351410   -0.19905889
   67    3     5.80600     2.70410     5.50115      0.00334419    1.22697929
0.00272555   -0.18849034
   68    3     4.99197     2.57363     4.97109      0.00453371    1.22697929
0.00369502   -0.18965214
   69    3     6.51267     3.70787     5.16387      0.00382539    1.34967722
0.00283430   -0.19061222
   70    3     6.38539     4.39517     4.26439      0.00415695    1.22697929
0.00338796   -0.19716603
   71    3     7.79137     3.47442     5.35900      0.00466349    1.71777100
0.00271485   -0.19281978
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   73    3     8.32318     0.02529     5.34341      0.00497067    1.22697929
0.00405114   -0.21156790
   74    3     7.26122    -0.31329     5.36499      0.00509304    1.22697929
0.00415088   -0.20979596
   75    3     5.23848     0.27926     4.99398      0.00642842    1.47237514
0.00436602   -0.20016939
   76    3     4.79686     1.31300     4.95091      0.00350992    0.85888550
0.00408660   -0.19338523
   77    3     5.47165     4.29232     3.49991      0.00501589    1.10428136
0.00454222   -0.20001838
   78    3     7.29150     4.81313     3.38270      0.00447435    1.10428136
0.00405182   -0.20770231
   79    3     8.53480     4.47698     3.52307      0.00576027    1.47237514
0.00391223   -0.20910291
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  718   16    -6.47572    -2.90198     2.81158     -0.00031033    0.24950915   -
0.00124377   -0.04972421
  719   16    -5.83282    -3.74421     2.42928     -0.00077581    0.55339050   -
0.00140193   -0.05066817
  720   16    -4.59222    -4.25979     2.20146     -0.00059972    0.55339050   -
0.00108372   -0.05727442
  721   16    -3.47270    -4.15000     2.26012     -0.00017226    0.24950915   -
0.00069038   -0.06433682
  722    9    -6.47287    -3.21110     2.29602     -0.00059955    0.54418906   -
0.00110173   -0.05015135
  723    9    -5.36066    -4.16070     1.86783     -0.00042843    0.54418906   -
0.00078728   -0.05553717
  724    9    -3.84449    -4.30343     1.81336     -0.00025049    0.54418906   -
0.00046030   -0.06427163
  725   17    -8.32131    -2.83317    -0.51537     -0.00072022    0.70628626   -
0.00101972   -0.04232684
  726   17    -8.33523    -2.61350     0.94878     -0.00266649    1.44729823   -
0.00184239   -0.03868311
  727    9    -7.37295    -3.28146     0.09128     -0.00100902    1.93355360   -
0.00052185   -0.04814419
  728    9    -7.36543    -2.87617     1.72176     -0.00000929    0.99623029   -
0.00000932   -0.05009989
  729   18    -5.21006     0.65429    -3.82188     -0.00125022    1.00790815   -
0.00124041   -0.07137050
  730    9    -4.66179    -0.29401    -3.59656      0.00027540    1.41970291
0.00019398   -0.08016108
  731   19    -5.42204     1.90174     3.28712     -0.00133972    1.04686146   -
0.00127974   -0.06930028
  732    9    -4.48021     1.29709     3.22809      0.00033896    1.47425008
0.00022992   -0.08521798
  733   15    -6.59314    -3.32072    -2.05210     -0.00058276    0.71934007   -
0.00081013   -0.05054302
  734   15    -5.87760    -2.48861    -3.07585     -0.00224890    1.47520770   -
0.00152446   -0.05390365
  735   10    -7.17410    -2.31598    -2.42167      0.00016508    1.96801831
0.00008388   -0.05633038
  736   10    -6.25336    -1.33360    -3.46452      0.00046869    1.01447461
0.00046200   -0.06452503
  737   16    -5.51260    -0.61548     3.88206     -0.00066897    0.72320223   -
0.00092501   -0.06085854
  738   16    -6.34101    -1.78066     3.39923     -0.00230471    1.48376859   -
0.00155328   -0.05077796
  739   10    -6.61939    -0.34301     3.45055      0.00031132    1.97799312
0.00015739   -0.06179367
  740   10    -7.45060    -1.67945     2.77608      0.00042922    1.01993340
0.00042083   -0.05463578
  741   17    -8.57122    -1.92351     1.96806     -0.00030650    0.24556786   -
0.00124814   -0.04317606
  742   17    -9.12118    -0.99009     2.25901     -0.00060281    0.54544158   -
0.00110518   -0.04369367
  743   17    -9.84953     0.09545     1.89491     -0.00061791    0.54544158   -
0.00113287   -0.04435754
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  744   17   -10.38131     0.72470     0.81662     -0.00061140    0.54544158   -
0.00112092   -0.04354131
  745   17   -10.49794     0.63901    -0.53265     -0.00072658    0.54544158   -
0.00133210   -0.04308915
  746   17   -10.15147    -0.12639    -1.59829     -0.00060690    0.54544158   -
0.00111267   -0.04383807
  747   17    -9.48432    -1.25690    -1.94228     -0.00060225    0.54544158   -
0.00110415   -0.04409852
  748   17    -8.77072    -2.28783    -1.42322     -0.00077767    0.54544158   -
0.00142576   -0.04244764
  749   10    -8.42568    -1.45573     2.30804     -0.00050282    0.53462138   -
0.00094051   -0.04732701
  750   10    -9.22488    -0.16819     2.38812     -0.00025356    0.53462138   -
0.00047427   -0.04952152
  751   10    -9.96874     0.84405     1.53667     -0.00015408    0.53462138   -
0.00028820   -0.04928846
  752   10   -10.35149     1.16491     0.10369     -0.00031128    0.53462138   -
0.00058224   -0.04819647
  753   10   -10.21581     0.66251    -1.32182     -0.00026078    0.53462138   -
0.00048779   -0.04856724
  754   10    -9.61748    -0.45664    -2.15392     -0.00018805    0.53462138   -
0.00035174   -0.04947753
  755   10    -8.80243    -1.73253    -2.05058     -0.00022488    0.53462138   -
0.00042063   -0.04867150
  756   10    -8.19627    -2.55894    -1.36446     -0.00006288    0.29765801   -
0.00021125   -0.04754957
  757   18    -6.20033     0.09225    -3.99846     -0.00026876    0.24971134   -
0.00107629   -0.06220518
  758   18    -7.33552     0.20913    -3.94640     -0.00058380    0.55730825   -
0.00104754   -0.05586351
  759   18    -8.42557     0.98036    -3.59575     -0.00050083    0.55730825   -
0.00089865   -0.05338598
  760   18    -8.75873     2.19941    -3.03995     -0.00052254    0.55730825   -
0.00093762   -0.05325995
  761   18    -8.19245     3.34467    -2.51681     -0.00062319    0.55730825   -
0.00111821   -0.05693156
  762   18    -6.96902     3.92614    -2.25016     -0.00053590    0.55730825   -
0.00096158   -0.06551068
  763   18    -5.61191     3.69502    -2.35410     -0.00053596    0.55730825   -
0.00096170   -0.07783561
  764   10    -6.64350    -0.25806    -3.79322     -0.00032900    0.54115976   -
0.00060796   -0.06124463
  765   10    -8.10510     0.19432    -3.58846     -0.00013437    0.54115976   -
0.00024830   -0.05722099
  766   10    -8.94708     1.37177    -3.05220     -0.00008117    0.54115976   -
0.00014999   -0.05574546
  767   10    -8.80916     2.77049    -2.41390     -0.00017885    0.54115976   -
0.00033049   -0.05753816
  768   10    -7.75038     3.79202    -1.94667     -0.00019411    0.54115976   -
0.00035869   -0.06406226
  769   10    -6.22373     3.99929    -1.85041     -0.00006530    0.54115976   -
0.00012067   -0.07636269
  770   10    -5.06103     3.56680    -2.04643      0.00003895    0.30268042
0.00012868   -0.09071283
  771   19    -5.21667     4.15771     0.81434     -0.00017161    0.25020996   -
0.00068586   -0.08405616
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  772   19    -6.26606     4.46347     0.47560     -0.00045818    0.55862443   -
0.00082019   -0.07154569
  773   19    -7.63546     4.32900     0.61273     -0.00050677    0.55862443   -
0.00090717   -0.06100345
  774   19    -8.59206     3.64943     1.34432     -0.00061015    0.55862443   -
0.00109223   -0.05474019
  775   19    -8.72519     2.71651     2.35629     -0.00046531    0.55862443   -
0.00083297   -0.05326502
  776   19    -7.97767     1.93077     3.21418     -0.00045960    0.55862443   -
0.00082274   -0.05481311
  777   19    -6.67045     1.62954     3.54968     -0.00068513    0.55862443   -
0.00122646   -0.05918741
  778   10    -5.48312     4.19921     0.27654     -0.00018438    0.54206154   -
0.00034015   -0.08428605
  779   10    -7.00007     4.39677     0.05224     -0.00009435    0.54206154   -
0.00017405   -0.06985244
  780   10    -8.37640     3.91509     0.56627     -0.00021114    0.54206154   -
0.00038951   -0.06028732
  781   10    -9.02120     2.96097     1.59796     -0.00017614    0.54206154   -
0.00032495   -0.05605900
  782   10    -8.65765     1.94402     2.70437     -0.00010757    0.54206154   -
0.00019845   -0.05637583
  783   10    -7.44184     1.30085     3.41051     -0.00021455    0.54206154   -
0.00039581   -0.05885783
  784   10    -6.19420     1.19554     3.53292     -0.00015315    0.30328480   -
0.00050497   -0.06492999
  785   16    -2.81305    -3.90888     2.72770     -0.00013029    0.90452236   -
0.00014404   -0.06817663
  786   16    -2.76910    -3.10693     3.67077     -0.00164106    1.80949903   -
0.00090691   -0.06550143
  787   16    -2.72887    -1.65380     4.04774     -0.00166688    1.80949903   -
0.00092118   -0.07140255
  788   13    -1.40208    -3.65646     3.07141     -0.00174384    1.80949903   -
0.00096372   -0.07448769
  789   13    -1.35163    -2.44427     3.95649     -0.00193066    1.80949903   -
0.00106696   -0.07600233
  790   13    -1.32618    -1.20603     3.97948     -0.00030164    0.90452236   -
0.00033348   -0.08585738
  791   15    -2.89604    -2.53581    -3.43371     -0.00018906    0.75162169   -
0.00025153   -0.07419037
  792   15    -2.87715    -3.54626    -3.12138     -0.00141498    1.50287454   -
0.00094151   -0.06611415
  793   15    -2.83622    -4.43641    -2.18193     -0.00125381    1.50287454   -
0.00083428   -0.06394530
  794   15    -2.79684    -4.69342    -1.15660     -0.00019807    0.75162169   -
0.00026353   -0.06718795
  795   14    -1.51636    -2.91792    -3.38948     -0.00136380    1.50287454   -
0.00090746   -0.07841371
  796   14    -1.48539    -4.05599    -2.77266     -0.00149297    1.50287454   -
0.00099341   -0.07269656
  797   14    -1.43854    -4.61028    -1.60339     -0.00114613    1.50287454   -
0.00076262   -0.07402064];
```

[$C_2H_6O_4P$] (Computation ID = 77)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.44
%   total number of segments         =    572
%   number of charge corr segments   =    296
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% P             0.88210708429032   -0.22071980418179    0.00000000000000   4.0062
0.0722    34.03     0.00212    6.4629
% O             1.89331650401399    0.21577762527952    3.26817828392488   3.2503
0.2017    40.08     0.00503    5.7070
% O             1.89331650401399    0.21577762527952   -3.26817828392488   3.2503
0.2021    40.20     0.00503    5.7070
% O            -1.19232275593831    2.31532186817995    0.00000000000000   3.2503
0.1815    49.14     0.00369    5.7070
% O            -0.76829919689687   -2.59709546996876    0.00000000000000   3.2503
0.3491    63.33     0.00551    5.7070
% C             0.03370308740605   -0.35491176097603    5.15043775780823   3.7795
0.0798    65.67     0.00122    6.2361
% C             0.03370308740605   -0.35491176097603   -5.15043775780823   3.7795
0.0799    65.67     0.00122    6.2361
% H            -0.71153316148603   -2.29337242459783    4.92153824813117   2.4566  -
0.0045    20.53    -0.00022    4.9133
% H            -1.58308467390722    0.97551684848296    5.07199111606339   2.4566  -
0.0071    21.79    -0.00033    4.9133
% H             0.93972422808295   -0.18880731554461    7.03226268264753   2.4566  -
0.0235    24.49    -0.00096    4.9133
% H            -1.58308467390722    0.97551684848296   -5.07199111606339   2.4566  -
0.0070    21.86    -0.00032    4.9133
% H            -0.71153316148603   -2.29337242459783   -4.92153824813117   2.4566  -
0.0049    20.60    -0.00024    4.9133
% H             0.93972422808295   -0.18880731554461   -7.03226268264753   2.4566  -
0.0234    24.49    -0.00096    4.9133
% H            -0.06573709967460    3.79408746068258    0.00000000000000   2.4566  -
0.0984    31.24    -0.00315    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -722.997001
%   Total energy + OC corr.      =       -723.003428
%   Dielectric energy            =         -0.104165      -2.834      -65.37
%   Diel. energy + OC corr.      =         -0.110592      -3.009      -69.40
%
```

```
%   Surface area of cavity [au]
acosmo =           523.111;
%   Total Volume of cavity [au]
vcosmo =           924.916;
%
%
% $screening_charge
%   cosmo           =    0.95963
%   corrected total =    0.99738
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1     3.49285     2.81766    -0.04738      0.00000493    1.11841584
0.00000441   -0.16212375
    2    1     4.81021    -0.88999     0.41476      0.00250835    1.11841584
0.00224277   -0.20471911
    3    1     2.92897    -3.54237    -0.90928      0.00115280    0.74561056
0.00154611   -0.21897789
    4    1     4.06533     2.17915    -0.39713      0.00086978    0.74561056
0.00116653   -0.18028023
    5    1     4.26931     1.89130     0.34092      0.00196658    1.11841584
0.00175836   -0.18508473
    6    1     4.83508     0.37175     0.27000      0.00280571    1.11841584
0.00250864   -0.20031079
    7    1     4.85090    -0.58898    -0.40371      0.00287386    1.11841584
0.00256958   -0.20441735
    8    1     3.11101    -3.54461     0.18319      0.00209315    0.93201320
0.00224584   -0.21508678
    9    1     2.75401    -3.43772     1.48211      0.00177330    0.74561056
0.00237832   -0.22220761
   10    1     2.68786    -3.36699    -1.70002      0.00148445    0.55920792
0.00265456   -0.22386090
   11    1     3.55604    -3.00087    -1.08199      0.00168542    1.11841584
0.00150697   -0.21050503
   12    1     3.95378    -2.78829    -0.14913      0.00108159    1.30481848
0.00082892   -0.20402841
   13    1     4.37393    -2.07254     0.65404      0.00240891    1.30481848
0.00184617   -0.20500711
   14    1     4.69036     0.98416    -0.30896      0.00240993    0.93201320
0.00258572   -0.19622683
   15    1     4.49198    -1.83392    -0.64521      0.00245799    1.49122112
0.00164830   -0.20494398
   16    1     3.56725    -3.04692     0.92326      0.00152196    1.30481848
0.00116642   -0.20939530
   17    2     4.78769    -1.17249     3.77802      0.00559208    0.98158343
0.00569700   -0.21567154
   18    2     4.32176     2.18023     4.16722      0.00633788    1.22697929
0.00516543   -0.19974191
   19    2     5.02263     0.11798     2.39501      0.00248012    0.61348964
0.00404265   -0.21582908
   20    2     5.01622    -0.61496     2.91898      0.00684777    1.10428136
0.00620111   -0.21815447
   21    2     4.72235     1.48929     2.29896      0.00412123    0.73618757
0.00559807   -0.20759182
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   22    2     4.69254     1.86185     3.12861      0.00603099    1.22697929
0.00491531   -0.20529211
   23    2     5.06937    -0.00594     3.92252      0.00632644    1.22697929
0.00515611   -0.20939838
   24    2     4.89654     1.13774     4.10203      0.00683678    1.34967722
0.00506549   -0.20371698
   25    2     3.86589     2.77833     3.59533      0.00603237    1.10428136
0.00546271   -0.20012678
   26    2     3.23577     3.17058     3.09022      0.00577113    0.85888550
0.00671933   -0.19738675
   27    2     4.52542    -1.65113     2.87923      0.00550906    1.10428136
0.00498882   -0.22396910
   28    2     4.71431    -0.64675     4.63299      0.00424361    0.85888550
0.00494083   -0.20462920
   29    2     4.36707    -0.41643     5.27953      0.00206880    0.49079171
0.00421523   -0.19360458
   30    2     4.25351     0.65592     5.45918      0.00293428    0.61348964
0.00478293   -0.18823223
   31    2     4.21506     1.57002     5.09582      0.00551595    1.10428136
0.00499506   -0.19187764
   32    2     3.46985     2.66768     4.70605      0.00406302    0.85888550
0.00473057   -0.19245496
   33    2     2.68756     3.05000     4.64699      0.00449445    0.73618757
0.00610503   -0.18923838
   34    2     2.16159     3.39268     3.90070      0.00376690    0.61348964
0.00614012   -0.19144052
   35    2     3.11434    -2.79413     3.38693      0.00274233    0.49079171
0.00558756   -0.22312940
   36    2     3.80133    -2.31690     3.98203      0.00312234    0.61348964
0.00508948   -0.21601748
   37    2     4.32200    -1.84208     3.92493      0.00441351    0.73618757
0.00599509   -0.21651259
   38    2     5.09256     0.71535     2.98545      0.00605174    1.22697929
0.00493222   -0.21076947
   39    2     4.00921     2.55605     2.48664      0.00568533    1.10428136
0.00514844   -0.20094839
   40    2     4.69084     0.42461     4.90981      0.00472843    0.98158343
0.00481715   -0.19789154
   41    2     2.92284     3.24199     3.85714      0.00426782    0.73618757
0.00579719   -0.19554889
   42    2     3.80304    -2.41308     3.18692      0.00516603    0.73618757
0.00701728   -0.22537328
   43    2     3.65387     2.08446     5.26147      0.00211078    0.61348964
0.00344060   -0.18708717
   44    2     4.24535    -1.44777     4.77324      0.00469732    0.85888550
0.00546909   -0.20363241
   45    3     3.36231     3.07933    -3.72279      0.00479909    0.85888550
0.00558757   -0.19768670
   46    3     4.99884     0.16890    -4.22631      0.00631436    1.22697929
0.00514626   -0.20621516
   47    3     4.14178    -2.12258    -3.06553      0.00471769    0.73618757
0.00640827   -0.22531724
   48    3     4.34244     2.13843    -2.33557      0.00366406    0.61348964
0.00597249   -0.20400768
   49    3     3.91624     2.71453    -2.79007      0.00566092    0.98158343
0.00576713   -0.20105958
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   50    3     4.93360     0.86168    -2.31737      0.00352576    0.73618757
0.00478921   -0.21133255
   51    3     5.12025     0.59127    -3.16592      0.00619381    1.22697929
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  533   11    -3.64866     0.17179    -4.00977     -0.00001706    0.24514070   -
0.00006961   -0.15741928
  534    7    -0.72594     3.28147    -5.53905     -0.00008651    0.53579899   -
0.00016146   -0.13595600
  535    7    -1.24849     2.72281    -6.83416      0.00005831    0.53579899
0.00010882   -0.12218227
  536    7    -2.14745     1.66445    -7.41229      0.00020228    0.53579899
0.00037753   -0.11618169
  537    7    -3.06306     0.52996    -7.04208     -0.00007935    0.53579899   -
0.00014810   -0.11742169
  538    7    -3.62889    -0.22666    -5.87168     -0.00007056    0.53579899   -
0.00013169   -0.13054287
  539    7    -3.61851    -0.30259    -4.36947      0.00012438    0.53579899
0.00023215   -0.15515427
  540   12    -3.10510    -2.53363    -4.43035      0.00003769    0.25564942
0.00014742   -0.15983145
  541   12    -2.97985    -2.71630    -5.56955     -0.00030968    0.57189208   -
0.00054150   -0.13656753
  542   12    -2.16453    -3.15404    -6.62215     -0.00038311    0.57189208   -
0.00066989   -0.12443820
  543   12    -0.88748    -3.67454    -6.87228     -0.00023235    0.57189208   -
0.00040629   -0.12545082
  544   12     0.28961    -4.04886    -6.20994     -0.00021742    0.57189208   -
0.00038018   -0.13616084
  545   12     0.84901    -4.11236    -4.92644     -0.00037292    0.57189208   -
0.00065209   -0.15825166
  546    7    -3.20229    -2.19273    -4.92432      0.00010381    0.55300257
0.00018772   -0.15080849
  547    7    -2.72215    -2.54837    -6.37287     -0.00008117    0.55300257   -
0.00014678   -0.12879251
  548    7    -1.48236    -3.11616    -7.14477      0.00000344    0.55300257
0.00000621   -0.12379076
  549    7    -0.02821    -3.64636    -6.90053      0.00008350    0.55300257
0.00015099   -0.13103766
  550    7     1.00070    -3.90578    -5.74756      0.00009563    0.55300257
0.00017293   -0.14849589
  551    7     1.27866    -3.86567    -4.50300      0.00010771    0.30987809
0.00034757   -0.17434209
  552   13     3.39337    -0.29857    -7.11138     -0.00016840    0.24736765   -
0.00068077   -0.13306629
  553   13     3.02919    -1.32447    -7.37725     -0.00051883    0.54836079   -
0.00094616   -0.12596016
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  554   13     2.06896    -2.11999    -7.90976     -0.00044573    0.54836079   -
0.00081283   -0.11733535
  555   13     0.84658    -2.09247    -8.49584     -0.00039343    0.54836079   -
0.00071746   -0.10948900
  556   13    -0.13995    -1.25312    -8.89673     -0.00048859    0.54836079   -
0.00089099   -0.10307676
  557   13    -0.48872     0.05611    -8.94910     -0.00051841    0.54836079   -
0.00094538   -0.10115399
  558   13    -0.05763     1.30183    -8.63161     -0.00041530    0.54836079   -
0.00075735   -0.10453364
  559   13     0.97767     1.97654    -8.07362     -0.00040432    0.54836079   -
0.00073732   -0.11074778
  560   13     2.19542     1.80536    -7.50244     -0.00048943    0.54836079   -
0.00089254   -0.12034938
  561   13     3.01574     1.11901    -7.16808     -0.00014920    0.24736765   -
0.00060315   -0.13016109
  562    7     3.35285    -0.80799    -6.79963     -0.00009977    0.53970879   -
0.00018486   -0.14217026
  563    7     2.60524    -2.04112    -7.26839     -0.00012277    0.53970879   -
0.00022747   -0.13032962
  564    7     1.31746    -2.49425    -7.92838      0.00005965    0.53970879
0.00011052   -0.12029157
  565    7     0.01416    -1.98278    -8.51071     -0.00006476    0.53970879   -
0.00011999   -0.11125368
  566    7    -0.77369    -0.71508    -8.77814     -0.00030871    0.53970879   -
0.00057199   -0.10534566
  567    7    -0.72512     0.79238    -8.62172     -0.00008579    0.53970879   -
0.00015896   -0.10714472
  568    7     0.14008     1.92548    -8.10517      0.00001648    0.53970879
0.00003054   -0.11321213
  569    7     1.46943     2.22257    -7.43894     -0.00014869    0.53970879   -
0.00027550   -0.12244714
  570    7     2.72134     1.56263    -6.89445     -0.00004381    0.53970879   -
0.00008117   -0.13709665
  571   14     0.17948     4.49066    -2.54761     -0.00025951    0.88980691   -
0.00029165   -0.13439795
  572    7     0.08112     3.63488    -4.21234      0.00268768    1.33353015
0.00201546   -0.16128950];
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[$MeSO_4$] (Computation ID = 78)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.33
%   total number of segments         =    596
%   number of charge corr segments   =    300
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% C            -4.99344506541626   -0.16944209835576    1.23462484715149   3.7795
0.0607    67.35     0.00090    6.2361
% O            -3.70753775287104    2.06084491497910    0.59441713773817   3.2503
0.2209    46.72     0.00473    5.7070
% S             0.05880616051654    1.18270513965225   -0.55933490324069   4.0818
0.0525    32.61     0.00161    6.5385
% O            -0.28470563721411   -1.06002512117250   -2.29979635585622   3.2503
0.2449    62.79     0.00390    5.7070
% O             0.76258374465887    3.63446878427064   -1.81123704203174   3.2503
0.2859    74.13     0.00386    5.7070
% O             3.04703780527958    0.32295265463462    1.27572254855689   3.2503
0.1911    43.95     0.00435    5.7070
% C             4.92781361664791   -0.68471549342086   -0.35027104950302   3.7795
0.0503    64.50     0.00078    6.2361
% H            -4.76616161566570   -0.71382701539421    3.25967736855535   2.4566  -
0.0144    26.10    -0.00055    4.9133
% H            -4.40747667208498   -1.79927040047810    0.04960764270312   2.4566  -
0.0071    18.12    -0.00039    4.9133
% H            -7.05115840940896    0.12796271006764    0.90271652151805   2.4566  -
0.0281    24.64    -0.00114    4.9133
% H             5.61377774471614    0.72658880267865   -1.74293810310850   2.4566  -
0.0148    23.43    -0.00063    4.9133
% H             4.25361051281312   -2.36596165981379   -1.40086255203490   2.4566  -
0.0119    20.28    -0.00059    4.9133
% H             6.54685556802894   -1.26228121764763    0.84767393955205   2.4566  -
0.0322    24.61    -0.00131    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -779.156244
%   Total energy + OC corr.      =       -779.161258
%   Dielectric energy            =         -0.099650      -2.712      -62.53
%   Diel. energy + OC corr.      =         -0.104663      -2.848      -65.68
%
%   Surface area of cavity [au]
acosmo =           529.231;
```

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%   Total Volume of cavity [au]
vcosmo =           917.724;
%
%
% $screening_charge
%   cosmo           =    0.96454
%   corrected total =    0.99790
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1    -5.56866     0.52767    -2.43518      0.00160754    0.82948843
0.00193799   -0.17493381
    2    1    -5.32864     2.28722     4.08713      0.00127174    0.66359074
0.00191646   -0.15585636
    3    1    -7.94504     0.05075     3.58490      0.00097519    0.82948843
0.00117565   -0.10959204
    4    1    -6.54680    -3.49403     2.13921      0.00027487    1.32718149
0.00020711   -0.10790644
    5    1    -2.81911    -3.13223     2.11689      0.00158775    1.32718149
0.00119633   -0.14547118
    6    1    -6.31105     1.05727    -2.08853      0.00062580    0.66359074
0.00094306   -0.16458758
    7    1    -7.03030     1.88356    -1.19862      0.00049301    0.33179537
0.00148589   -0.15265713
    8    1    -6.67826     0.17891    -2.13053      0.00109640    1.49307918
0.00073432   -0.14639824
    9    1    -7.08761    -0.73705    -1.85997      0.00105927    1.16128380
0.00091216   -0.13232823
   10    1    -5.63250    -0.36172    -2.48544      0.00068681    0.82948843
0.00082799   -0.16147121
   11    1    -5.84657    -1.02577    -2.34631      0.00080627    0.82948843
0.00097200   -0.15018667
   12    1    -3.31466    -3.10296     2.92590      0.00096914    0.66359074
0.00146044   -0.13513562
   13    1    -6.26615    -3.20328     3.09477      0.00046036    1.16128380
0.00039643   -0.10757061
   14    1    -7.35330    -0.01004     4.18248      0.00147005    1.32718149
0.00110765   -0.11261391
   15    1    -5.49834     1.67900     4.49232      0.00054148    0.66359074
0.00081598   -0.13926749
   16    1    -7.46977    -2.11778    -0.85246      0.00138612    1.16128380
0.00119361   -0.11769341
   17    1    -6.84087    -2.34620    -1.24185      0.00110393    0.82948843
0.00133085   -0.12458223
   18    1    -6.24975     2.10589     3.97850      0.00091319    1.16128380
0.00078637   -0.14046531
   19    1    -7.49151     1.23173     3.70051      0.00129738    1.32718149
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   20    1    -7.89491    -1.21707     3.41822      0.00153349    1.82487455
0.00084033   -0.10440563
   21    1    -7.36041    -2.65626     2.81491      0.00045585    1.49307918
0.00030531   -0.10347941
   22    1    -5.33836    -3.84297     2.05340      0.00091943    1.49307918
0.00061579   -0.11612986
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   23    1    -3.96065    -3.63633     2.32925      0.00161582    1.32718149
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   25    1    -4.48779     2.00422     4.28484      0.00107759    0.49769306
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   26    1    -6.58085     2.65681     3.17800      0.00135674    0.99538612
0.00136302   -0.14792438
   27    1    -7.18659     2.80784     2.01574      0.00087821    1.16128380
0.00075624   -0.14411162
   28    1    -7.83459    -2.54807     0.49025      0.00064295    1.32718149
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   29    1    -7.33829    -3.12879     1.40205      0.00038994    1.65897686
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   30    1    -6.24708    -3.73230     1.09851      0.00049127    0.99538612
0.00049354   -0.11212832
   31    1    -6.87134     1.34835    -1.67296      0.00074349    0.66359074
0.00112040   -0.15242099
   32    1    -6.68380    -1.53715    -1.85669      0.00142750    1.16128380
0.00122925   -0.13358141
   33    1    -2.31761    -1.79227     3.35374      0.00014219    0.16589769
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   34    1    -4.90982    -3.55724     2.90794      0.00105551    1.16128380
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   35    1    -7.26197    -2.07707     3.57959      0.00075883    0.99538612
0.00076234   -0.10458997
   36    1    -6.66159     1.20616     4.33450      0.00114162    1.16128380
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   37    1    -3.57270     1.50552     4.31039      0.00049730    0.49769306
0.00099921   -0.16447801
   38    1    -7.01064    -3.14608     0.07074      0.00133276    1.49307918
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   39    1    -7.39199     2.11221     3.05816      0.00106956    1.32718149
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   40    1    -8.00390    -2.28636     2.09480      0.00021940    1.16128380
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   41    2    -3.39242     4.36324     2.86697      0.00615034    1.10428136
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   42    2    -5.40771     4.81203     0.27021      0.00514246    1.22697929
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   43    2    -4.37745     3.10489    -2.40988      0.00551763    0.98158343
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   44    2    -2.89564     5.13029     1.29020      0.00221833    0.49079171
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   45    2    -2.99165     4.88635     2.03275      0.00665767    1.22697929
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   46    2    -3.65199     5.26862     0.07303      0.00294414    0.61348964
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   47    2    -4.40449     5.17004    -0.04736      0.00393092    0.98158343
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   48    2    -2.58675     3.99293     2.95570      0.00542711    0.98158343
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   50    2    -4.94369     4.99338     1.25541      0.00658155    1.47237514
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   51    2    -5.26784     4.55690    -0.78394      0.00578549    1.34967722
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   58    2    -6.23561     4.00551    -0.03152      0.00472980    1.22697929
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   59    2    -6.23692     3.49517    -0.85802      0.00378421    0.85888550
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   62    2    -4.49499     2.11535    -2.55860      0.00441873    0.73618757
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   63    2    -3.80454     5.27786     1.04850      0.00594478    1.34967722
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   64    2    -4.21293     4.78713    -1.10165      0.00627175    1.34967722
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   65    2    -2.40070     2.79183     3.47931      0.00526090    0.85888550
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   66    2    -5.53099     4.25261     2.15518      0.00554614    1.34967722
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   70    3    -0.18808    -1.81592     2.19903     -0.00008839    0.38700612   -
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   73    3     1.02533     4.24264     1.96332      0.00082767    0.96751531
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   74    3    -2.19298     2.06405    -3.84777      0.00093694    0.77401224
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   75    3     0.22226     3.48463     2.80751     -0.00057239    1.54802449   -
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   77    3    -0.43830     2.47540     3.28034      0.00042104    0.77401224
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0.00031023   -0.19854563
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79	3	-2.67631	1.86037	-3.51249	0.00082679	0.77401224
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81	4	1.38620	-1.13122	-5.08685	0.00451343	0.98158343
0.00459811	-0.20252635					
82	4	-1.92244	-0.59527	-5.06865	0.00505610	1.22697929
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83	4	-0.69420	-3.98169	-0.93565	0.00413003	0.85888550
0.00480859	-0.19365553					
84	4	0.45512	-3.84189	-3.80931	0.00480262	1.47237514
0.00326182	-0.18298531					
85	4	0.21244	-2.98298	-4.87270	0.00412766	1.34967722
0.00305826	-0.18679572					
86	4	0.79405	-2.12243	-5.17596	0.00393531	1.10428136
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87	4	-1.20695	-2.72327	-4.93568	0.00433265	1.47237514
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88	4	-1.84052	-1.74516	-5.07013	0.00470620	1.34967722
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89	4	-1.72218	-3.46610	-3.94578	0.00383634	1.34967722
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90	4	-2.46286	-3.15354	-3.49880	0.00327853	0.85888550
0.00381719	-0.18793860					
91	4	-0.73424	-4.13249	-3.26035	0.00414621	1.47237514
0.00281600	-0.18269578					
92	4	-0.64561	-4.28572	-2.12836	0.00385223	1.10428136
0.00348845	-0.18673699					
93	4	1.61865	-1.94412	-4.78180	0.00372864	0.73618757
0.00506480	-0.19575253					
94	4	0.34529	-1.01511	-5.48818	0.00488012	1.22697929
0.00397734	-0.20339591					
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0.00017025   -0.14837267
  578   13     6.07751    -1.75125     3.21099     -0.00025735    0.24140576   -
0.00106603   -0.11827370
  579   13     6.10292    -2.72370     2.70777     -0.00072084    0.53249775   -
0.00135370   -0.10987029
  580   13     6.54888    -3.50153     1.73001     -0.00064867    0.53249775   -
0.00121817   -0.10124578
  581   13     7.33122    -3.52985     0.65900     -0.00064438    0.53249775   -
0.00121011   -0.09392592
  582   13     8.14606    -2.79766    -0.08923     -0.00076647    0.53249775   -
0.00143939   -0.08863153
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  583   13     8.67688    -1.58937    -0.22406     -0.00074814    0.53249775   -
0.00140496   -0.08849392
  584   13     8.71749    -0.37431     0.30690     -0.00064732    0.53249775   -
0.00121564   -0.09375872
  585   13     8.25212     0.37553     1.29740     -0.00062849    0.53249775   -
0.00118026   -0.10140106
  586   13     7.46153     0.36890     2.36270     -0.00070800    0.53249775   -
0.00132958   -0.11048221
  587   13     6.77639    -0.16040     3.03347     -0.00022601    0.24140576   -
0.00093624   -0.11856533
  588    7     5.64687    -2.11343     3.02734     -0.00052850    0.52915788   -
0.00099876   -0.12573947
  589    7     5.87188    -3.29235     2.15480     -0.00035179    0.52915788   -
0.00066481   -0.11323564
  590    7     6.59482    -3.76683     0.94897     -0.00016224    0.52915788   -
0.00030660   -0.10383355
  591    7     7.53487    -3.35256    -0.12178     -0.00029101    0.52915788   -
0.00054995   -0.09597426
  592    7     8.32688    -2.21045    -0.64152     -0.00054199    0.52915788   -
0.00102425   -0.09175929
  593    7     8.66320    -0.78415    -0.40837     -0.00031822    0.52915788   -
0.00060137   -0.09563534
  594    7     8.41320     0.37232     0.48711     -0.00025123    0.52915788   -
0.00047477   -0.10378027
  595    7     7.67399     0.80975     1.69708     -0.00033039    0.52915788   -
0.00062437   -0.11393943
  596    7     6.73269     0.35822     2.75154     -0.00042719    0.52915788   -
0.00080731   -0.12601996];
```

[C8SO4] (Computation ID = 80)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.33
%   total number of segments         =   1176
%   number of charge corr segments   =    468
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% S           -11.59597986609543   -0.49379495507431    0.08804236113941   4.0818
0.0566    28.50     0.00199    6.5385
% O            -8.72744025588589    1.10017266066036    0.15064584126645   3.2503
0.1471    37.78     0.00389    5.7070
% O           -11.58038136368161   -1.83290153702389   -2.39826223238410   3.2503
0.2852    71.68     0.00398    5.7070
% O           -13.36287718880228    1.67759670834008    0.29520767128999   3.2503
0.2926    75.19     0.00389    5.7070
% O           -11.47520462351954   -2.20685579272745    2.33036288776629   3.2503
0.2823    70.72     0.00399    5.7070
% C             0.65343681267739    0.89444731992730   -0.06372542923574   3.7795
0.0173    20.07     0.00086    6.2361
% C             3.06100398110089   -0.71805969962101    0.01623986809070   3.7795
0.0187    20.41     0.00092    6.2361
% C            -1.79895728048109   -0.64731667396538    0.03617532975590   3.7795
0.0142    20.35     0.00070    6.2361
% C             5.51198716505020    0.82516248253876   -0.08896074120205   3.7795
0.0186    20.05     0.00093    6.2361
% C            -4.19885820607098    0.97582214318339   -0.01810758230785   3.7795
0.0142    21.45     0.00066    6.2361
% C             7.92230873591252   -0.78188215136443    0.00589268970084   3.7795
0.0229    26.03     0.00088    6.2361
% C            -6.61830060999546   -0.59253714376570    0.09650233240921   3.7795
0.0157    24.33     0.00065    6.2361
% C            10.35826549423784    0.78002194452525   -0.10107732874426   3.7795
0.0587    58.68     0.00100    6.2361
% H             0.66318453592534    2.06344340550099   -1.79531602743011   2.4566  -
0.0117    25.62    -0.00046    4.9133
% H             0.68024117747337    2.24594013632959    1.52877188886683   2.4566  -
0.0123    25.31    -0.00049    4.9133
% H             3.03587899134576   -2.07881661111271   -1.56823682683805   2.4566  -
0.0112    25.45    -0.00044    4.9133
% H             3.05256579081441   -1.87741054179451    1.75440165440322   2.4566  -
0.0110    25.38    -0.00043    4.9133
% H            -1.80117594556348   -1.82137145244074    1.76425427067918   2.4566  -
0.0147    25.32    -0.00058    4.9133
```

```
% H            -1.82931527336539   -1.99292409141919   -1.56089803574739   2.4566  -
0.0155    25.44    -0.00061    4.9133
% H             5.53591997950541    2.18957461946444    1.49286069387930   2.4566  -
0.0105    25.63    -0.00041    4.9133
% H             5.52589195129161    1.98174038028069   -1.82925048574295   2.4566  -
0.0106    25.47    -0.00042    4.9133
% H            -4.23379774545903    2.14415501425570   -1.74658119064261   2.4566  -
0.0182    25.68    -0.00071    4.9133
% H            -4.18829452931788    2.30798306321672    1.58785638147515   2.4566  -
0.0181    25.46    -0.00071    4.9133
% H             7.90296954142127   -2.14708503851794   -1.57278314317764   2.4566  -
0.0136    25.23    -0.00054    4.9133
% H             7.91175329836534   -1.93177372375487    1.74843045244003   2.4566  -
0.0138    25.01    -0.00055    4.9133
% H            -6.75647519784186   -1.84921818260835   -1.56835170895836   2.4566  -
0.0156    21.20    -0.00074    4.9133
% H            -6.63355718725394   -1.80035847460825    1.80285136931297   2.4566  -
0.0153    21.37    -0.00071    4.9133
% H            10.46752170712841    1.89351324379947   -1.85932234952549   2.4566  -
0.0168    25.04    -0.00067    4.9133
% H            12.05253465530883   -0.42937710165151   -0.01751352611347   2.4566  -
0.0204    24.43    -0.00083    4.9133
% H            10.46515145577517    2.12211004942745    1.48989091557455   2.4566  -
0.0166    24.98    -0.00067    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =      -1014.569012
%   Total energy + OC corr.      =      -1014.573828
%   Dielectric energy            =         -0.106461      -2.897      -66.81
%   Diel. energy + OC corr.      =         -0.111277      -3.028      -69.83
%
%   Surface area of cavity [au]  =           917.285
%   Total Volume of cavity [au]  =          1730.255
%
%
% $screening_charge
%   cosmo           =    0.95083
%   corrected total =    0.99820
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1   -13.87263    -3.86965    -0.19734      0.00130827    0.58050918
0.00225367   -0.21592761
    2    1   -11.74590     1.21847     3.79032      0.00085380    0.38700612
0.00220616   -0.22243323
    3    1   -11.17763     2.10019    -3.03566      0.00070041    0.58050918
0.00120654   -0.21648321
    4    1   -15.25011    -1.70219     1.44749      0.00055538    0.77401224
0.00071753   -0.21021537
    5    1   -11.20035     1.82834     3.42156      0.00111226    0.77401224
0.00143700   -0.21716638
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    6    1   -11.87007     1.91578    -3.19526      0.00095895    0.58050918
0.00165191   -0.22228577
    7    1   -15.34748    -1.30339    -1.30187      0.00077357    1.35452143
0.00057110   -0.21118811
    8    1   -15.54835    -1.48786     0.31511      0.00074020    1.16101837
0.00063754   -0.20474018
    9    1   -15.00058    -1.14840     2.24239      0.00133892    0.38700612
0.00345970   -0.22208708
   10    1   -10.67283     1.19715     3.68662      0.00043763    0.19350306
0.00226164   -0.21521587
   11    1   -10.71741     1.91431    -3.08850      0.00088686    0.38700612
0.00229159   -0.21578859
   12    1   -14.63503    -3.20911    -0.14041      0.00048123    1.35452143
0.00035528   -0.20459954
   13    1   -15.08308    -2.54298     0.63756      0.00017087    1.54802449
0.00011038   -0.20160717
   14    1   -10.67216     1.59772     3.46936      0.00023882    0.19350306
0.00123420   -0.21500127
   15    1   -15.19862    -2.26365    -0.65329      0.00015010    1.54802449
0.00009696   -0.20162360
   16    2    -8.60658     3.48601    -2.05340      0.00427764    0.85888550
0.00498046   -0.20089372
   17    2    -8.22695     4.09747     1.30413      0.00475581    1.10428136
0.00430670   -0.19320061
   18    2    -9.23980     2.27507     3.13760      0.00231596    0.61348964
0.00377506   -0.21096790
   19    2    -9.33277     3.83793    -1.49341      0.00361650    0.85888550
0.00421069   -0.20959901
   20    2    -9.24504     4.21315     0.92926      0.00478523    1.22697929
0.00390001   -0.20693609
   21    2    -8.66554     4.15564    -0.95614      0.00294446    0.73618757
0.00399961   -0.19990291
   22    2    -8.39839     4.33338     0.20379      0.00420008    1.10428136
0.00380345   -0.19511216
   23    2    -8.64176     3.71575     2.07840      0.00502190    1.10428136
0.00454766   -0.20047390
   24    2    -9.25707     2.88102     2.81764      0.00352903    0.73618757
0.00479365   -0.21063552
   25    2    -9.44239     3.15649    -2.26286      0.00381034    0.73618757
0.00517577   -0.21260896
   26    2    -8.15932     3.88881    -1.41952      0.00284503    0.61348964
0.00463745   -0.19335710
   27    2    -8.23822     2.31058     3.12728      0.00357728    0.73618757
0.00485920   -0.19534521
   28    2    -8.65953     1.63894     3.35531      0.00332039    0.61348964
0.00541229   -0.20227363
   29    2    -8.42964     2.01972    -2.95263      0.00254841    0.49079171
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   30    2    -8.61556     2.77960    -2.62993      0.00333600    0.73618757
0.00453145   -0.20206412
   31    2    -9.32247     4.26453    -0.29374      0.00419398    0.98158343
0.00427267   -0.20790946
   32    2    -9.41491     3.58077     2.13529      0.00288094    0.73618757
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   33    2    -7.97685     4.18266    -0.55618      0.00186416    0.49079171
0.00379826   -0.18974251
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   34    2    -8.38086     3.03455     2.73964      0.00389025    0.85888550
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0.00470569   -0.20982704
   36    3   -11.58284    -3.29175    -5.30280      0.00358864    1.34967722
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   37    3    -9.62224    -0.76794    -4.76386      0.00371801    0.73618757
0.00505036   -0.20384908
   38    3   -12.63573    -0.26235    -5.04102      0.00478673    1.10428136
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   39    3   -14.43680    -2.76602    -3.63716      0.00526209    1.22697929
0.00428865   -0.21472688
   40    3   -12.21351    -5.02027    -2.46545      0.00505985    1.22697929
0.00412383   -0.21289220
   41    3   -10.61635    -2.57840    -5.41147      0.00417840    1.47237514
0.00283786   -0.19203903
   42    3   -10.12715    -1.49322    -5.28569      0.00304609    0.85888550
0.00354656   -0.19816119
   43    3   -11.98369    -2.21124    -5.60120      0.00429290    1.47237514
0.00291563   -0.19641852
   44    3   -12.34199    -1.11891    -5.47637      0.00448773    1.22697929
0.00365755   -0.20601381
   45    3   -12.76592    -3.30380    -5.04318      0.00419215    1.47237514
0.00284720   -0.19668627
   46    3   -13.71577    -3.30837    -4.35474      0.00463133    1.34967722
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   47    3   -11.87871    -4.20560    -4.59960      0.00390474    1.34967722
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   48    3   -11.98669    -4.80925    -3.63960      0.00425944    1.22697929
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   49    3   -10.62201    -3.85389    -4.75659      0.00482225    1.71777100
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   50    3    -9.77345    -3.97217    -4.04843      0.00468833    1.22697929
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   51    3   -10.45444    -0.38308    -5.08057      0.00506123    1.22697929
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   53    3   -13.51112    -0.93793    -4.85507      0.00597701    1.47237514
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   54    3   -14.20587    -1.92426    -4.31220      0.00580570    1.47237514
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   55    3   -14.00265    -3.84744    -3.19761      0.00604479    1.47237514
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   56    3   -13.17582    -4.63003    -2.84027      0.00585768    1.47237514
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   57    3   -11.12496    -5.04676    -2.56669      0.00559858    1.34967722
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   58    3   -10.06099    -4.65284    -2.94962      0.00598123    1.34967722
0.00443160   -0.20276248
   59    3    -9.53457    -1.93804    -4.92178      0.00311176    0.85888550
0.00362302   -0.19513166
   60    3   -10.04954     0.19334    -4.42691      0.00378590    0.73618757
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   61    3   -12.09146     0.60746    -4.48346      0.00594217    1.22697929
0.00484293   -0.22465873
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   62    3   -13.23698     0.18304    -4.33637      0.00495716    1.10428136
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   65    3   -12.87666    -4.71129    -1.62412      0.00520041    1.10428136
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   66    3   -11.56181    -4.98046    -1.58756      0.00434092    0.85888550
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   67    3   -11.08634    -1.33265    -5.57162      0.00493644    1.47237514
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   68    3   -13.25752    -2.19142    -5.15929      0.00558813    1.71777100
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   69    3   -12.99340    -4.27082    -4.01832      0.00481752    1.47237514
0.00327194   -0.20199706
   70    3   -10.88551    -4.70306    -3.75618      0.00463605    1.34967722
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   71    3    -9.67302    -2.91537    -4.79716      0.00413763    1.10428136
0.00374690   -0.19170615
   72    3   -10.90673     0.56563    -4.48579      0.00517193    1.10428136
0.00468353   -0.21979377
   73    3   -14.26366    -0.81103    -3.92158      0.00670353    1.34967722
0.00496677   -0.22453831
   74    3   -13.88361    -4.08602    -1.97005      0.00603556    1.22697929
0.00491904   -0.22012947
   75    3   -10.32033    -4.75697    -1.74503      0.00622669    1.10428136
0.00563868   -0.21450255
   76    4   -15.48116     4.13292     0.51625      0.00347084    1.34967722
0.00257161   -0.19883112
   77    4   -15.74230     1.47352     2.50005      0.00451614    1.10428136
0.00408966   -0.21871887
   78    4   -16.40360     1.18633    -0.74276      0.00515114    1.22697929
0.00419823   -0.21740505
   79    4   -14.27298     3.18833    -2.43500      0.00463202    1.10428136
0.00419460   -0.21999206
   80    4   -12.23824     4.67315    -0.27605      0.00490088    1.22697929
0.00399427   -0.21808327
   81    4   -12.97633     3.60207     2.88586      0.00427356    0.98158343
0.00435374   -0.21998408
   82    4   -15.80048     3.47484     1.47528      0.00410601    1.47237514
0.00278870   -0.20173704
   83    4   -15.93348     2.46180     2.12323      0.00463729    1.34967722
0.00343585   -0.20951726
   84    4   -16.19311     3.26598     0.11785      0.00409763    1.47237514
0.00278301   -0.20167514
   85    4   -16.51707     2.22484    -0.26716      0.00420242    1.22697929
0.00342501   -0.20870120
   86    4   -15.30378     4.09499    -0.68138      0.00412110    1.47237514
0.00279895   -0.20193205
   87    4   -14.72085     3.87668    -1.67572      0.00468564    1.34967722
0.00347167   -0.20983413
   88    4   -14.49914     4.72098     0.18916      0.00372715    1.34967722
0.00276151   -0.20120726
   89    4   -13.38877     4.91668     0.02655      0.00399118    1.22697929
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92	4	-16.32815	1.31462	1.57586	0.00481073	1.22697929
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93	4	-16.57738	1.21739	0.43633	0.00528308	1.34967722
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94	4	-16.07953	1.87008	-1.47891	0.00583097	1.47237514
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95	4	-15.23995	2.60309	-2.19171	0.00580567	1.47237514
0.00394306	-0.21769762					
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 1053   24     9.10094    -1.52565    -3.65182     -0.00024873    0.74226103   -
0.00033510   -0.04279219
 1054   24     9.86650    -2.58587    -2.82035     -0.00141581    1.52632924   -
0.00092759   -0.03938356
 1055   13    10.23014    -1.23058    -3.28848      0.00133520    2.02707518
0.00065869   -0.04757537
 1056   13    10.98271    -2.40180    -2.21455      0.00103702    1.04689009
0.00099057   -0.04666956
 1057   25    10.09723    -2.64494     2.67460     -0.00016233    0.74358828   -
0.00021831   -0.04211187
 1058   25     9.44799    -1.49899     3.49603     -0.00145568    1.52927287   -
0.00095188   -0.03971918
 1059   13    10.74257    -1.61251     2.78727      0.00133194    2.03051352
0.00065596   -0.04687643
 1060   13     9.88801    -0.29632     3.58671      0.00098482    1.04876034
0.00093903   -0.04817967
 1061   28     9.45063     4.13051    -1.85346     -0.00007798    0.24339511   -
0.00032038   -0.04480933
 1062   28    10.53900     4.28984    -1.68493     -0.00028726    0.53967910   -
0.00053228   -0.04242726
 1063   28    11.81162     3.88631    -1.86140     -0.00036229    0.53967910   -
0.00067130   -0.04018267
 1064   28    12.56487     2.92266    -2.42487     -0.00035593    0.53967910   -
0.00065953   -0.03921955
 1065   28    12.49420     1.78850    -3.14751     -0.00022108    0.53967910   -
0.00040965   -0.03948418
 1066   28    11.62818     0.94241    -3.73715     -0.00028752    0.53967910   -
0.00053277   -0.03963025
 1067   28    10.31696     0.72649    -3.95536     -0.00049717    0.53967910   -
0.00092123   -0.03933797
 1068   13     9.77023     4.24415    -1.36607      0.00006499    0.53074639
0.00012246   -0.04758151
 1069   13    11.27420     4.19475    -1.30389      0.00017423    0.53074639
0.00032828   -0.04539256
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 1070   13    12.46903     3.38842    -1.74029      0.00000030    0.53074639
0.00000056   -0.04312570
 1071   13    12.87160     2.15116    -2.49882      0.00010683    0.53074639
0.00020129   -0.04305090
 1072   13    12.31916     0.98325    -3.27278      0.00006541    0.53074639
0.00012324   -0.04350448
 1073   13    11.03506     0.35690    -3.74924     -0.00001855    0.53074639   -
0.00003496   -0.04306072
 1074   13     9.81369     0.36349    -3.82096      0.00004877    0.29502437
0.00016531   -0.04387281
 1075   29    12.07140    -2.45857    -1.40080     -0.00016346    0.25010525   -
0.00065358   -0.03778556
 1076   29    12.66255    -1.67029    -1.97830     -0.00043399    0.55792890   -
0.00077786   -0.03699200
 1077   29    13.46358    -0.54646    -1.95449     -0.00035719    0.55792890   -
0.00064021   -0.03725286
 1078   29    14.05722     0.34531    -1.08413     -0.00041242    0.55792890   -
0.00073919   -0.03643992
 1079   29    14.19000     0.62424     0.26114     -0.00045077    0.55792890   -
0.00080793   -0.03622065
 1080   29    13.80522     0.17124     1.50691     -0.00035538    0.55792890   -
0.00063697   -0.03711177
 1081   29    13.06717    -0.82027     2.12123     -0.00037547    0.55792890   -
0.00067297   -0.03724258
 1082   29    12.29101    -1.92693     1.84179     -0.00049951    0.55792890   -
0.00089529   -0.03679813
 1083   13    11.93945    -2.10114    -1.86627     -0.00010790    0.54229007   -
0.00019898   -0.04093781
 1084   13    12.80747    -0.91817    -2.34488      0.00000463    0.54229007
0.00000854   -0.04165086
 1085   13    13.63246     0.27411    -1.81595      0.00010685    0.54229007
0.00019703   -0.04158145
 1086   13    14.06216     0.96662    -0.50534     -0.00001964    0.54229007   -
0.00003622   -0.04049994
 1087   13    13.91309     0.86365     1.02734     -0.00003797    0.54229007   -
0.00007003   -0.04091721
 1088   13    13.24890     0.00918     2.12764      0.00009433    0.54229007
0.00017394   -0.04200785
 1089   13    12.35320    -1.23195     2.32573     -0.00004198    0.54229007   -
0.00007741   -0.04115534
 1090   13    11.69950    -2.18203     1.82918     -0.00004657    0.30315788   -
0.00015360   -0.04165081
 1091   30     9.88795     1.28266     3.72606     -0.00011558    0.24336453   -
0.00047491   -0.04081390
 1092   30    10.99887     1.26094     3.66972     -0.00037057    0.53957374   -
0.00068679   -0.03945900
 1093   30    12.14509     1.76101     3.17083     -0.00027030    0.53957374   -
0.00050094   -0.03954457
 1094   30    12.63601     2.70283     2.34333     -0.00028454    0.53957374   -
0.00052734   -0.03938311
 1095   30    12.27323     3.70581     1.52162     -0.00032266    0.53957374   -
0.00059798   -0.03969168
 1096   30    11.20336     4.36462     1.03775     -0.00026692    0.53957374   -
0.00049469   -0.04143706
 1097   30     9.85874     4.41304     1.08728     -0.00021244    0.53957374   -
0.00039373   -0.04334693
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 1098   13    10.27779     0.84477     3.63200     -0.00019195    0.53071657   -
0.00036169   -0.04291023
 1099   13    11.74309     1.05489     3.35626      0.00004650    0.53071657
0.00008761   -0.04352523
 1100   13    12.70862     1.90527     2.57400      0.00012034    0.53071657
0.00022675   -0.04333017
 1101   13    12.78419     3.05224     1.60135      0.00002690    0.53071657
0.00005068   -0.04301324
 1102   13    11.93926     4.03231     0.83137      0.00008950    0.53071657
0.00016864   -0.04410295
 1103   13    10.51528     4.44941     0.57521      0.00014508    0.53071657
0.00027336   -0.04695578
 1104   13     9.31643     4.30944     0.77386      0.00021943    0.29498730
0.00074387   -0.04896900
 1105   21     3.82664     1.82255    -3.89410      0.00021357    0.87926480
0.00024290   -0.05429667
 1106   21     3.84722     2.92864    -3.60681     -0.00041688    1.75757580   -
0.00023719   -0.05189682
 1107   21     3.87018     3.87018    -2.58207     -0.00009245    1.75757580   -
0.00005260   -0.05539510
 1108   14     2.33497     2.27812    -3.80364     -0.00032427    1.75757580   -
0.00018450   -0.05713218
 1109   14     2.36019     3.51605    -3.16804     -0.00044164    1.75757580   -
0.00025128   -0.05741541
 1110   14     2.37668     4.08680    -2.17790      0.00033501    0.87926480
0.00038101   -0.06292306
 1111   22    -2.51102     4.16135    -2.14414      0.00020864    0.87279286
0.00023905   -0.08637732
 1112   22    -2.53007     3.59624    -3.12106     -0.00061922    1.74450882   -
0.00035496   -0.08097303
 1113   22    -2.55650     2.37587    -3.75491     -0.00060469    1.74450882   -
0.00034663   -0.08104396
 1114   14    -1.00675     3.94661    -2.54730     -0.00023431    1.74450882   -
0.00013431   -0.07447236
 1115   14    -1.03217     3.01710    -3.56078     -0.00052660    1.74450882   -
0.00030186   -0.07120321
 1116   14    -1.05304     1.92683    -3.85227      0.00015874    0.87279286
0.00018188   -0.07383518
 1117   20     3.88171     4.29133     1.63026      0.00034813    0.87976714
0.00039571   -0.05833458
 1118   20     3.88426     3.84049     2.68276     -0.00039953    1.75860565   -
0.00022719   -0.05279587
 1119   20     3.87658     2.68353     3.46059     -0.00029748    1.75860565   -
0.00016916   -0.05239170
 1120   15     2.38607     4.16480     2.05569     -0.00011482    1.75860565   -
0.00006529   -0.05998455
 1121   15     2.38496     3.34890     3.18615     -0.00046804    1.75860565   -
0.00026614   -0.05644282
 1122   15     2.37565     2.28201     3.60170      0.00020498    0.87976714
0.00023300   -0.05887922
 1123   23    -2.47901     2.32230     3.65157      0.00006949    0.87420176
0.00007949   -0.08273666
 1124   23    -2.47031     3.38557     3.25211     -0.00080428    1.74741672   -
0.00046027   -0.07990731
 1125   23    -2.47321     4.21375     2.14370     -0.00034966    1.74741672   -
0.00020010   -0.08330038
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 1126   15    -0.97373     2.72001     3.50918     -0.00042671    1.74741672   -
0.00024420   -0.07168918
 1127   15    -0.96815     3.87880     2.75310     -0.00055108    1.74741672   -
0.00031537   -0.07177405
 1128   15    -0.97478     4.34501     1.71735      0.00025907    0.87420176
0.00029635   -0.07722289
 1129   19    -0.15095    -2.07631    -3.64756      0.00014391    0.87829050
0.00016385   -0.06862552
 1130   19    -0.16911    -3.14045    -3.23531     -0.00060722    1.75561648   -
0.00034587   -0.06612552
 1131   19    -0.18184    -3.95759    -2.11102     -0.00027478    1.75561648   -
0.00015651   -0.06957860
 1132   16     1.34219    -2.52046    -3.52091     -0.00030602    1.75561648   -
0.00017431   -0.06076924
 1133   16     1.32296    -3.67569    -2.74826     -0.00041444    1.75561648   -
0.00023606   -0.06114758
 1134   16     1.31653    -4.12921    -1.70090      0.00033754    0.87829050
0.00038432   -0.06666143
 1135   24     6.19059    -4.20453    -1.68743      0.00034952    0.87948836
0.00039742   -0.05191264
 1136   24     6.19585    -3.75970    -2.73972     -0.00036712    1.75801084   -
0.00020883   -0.04652689
 1137   24     6.21125    -2.60960    -3.52232     -0.00033059    1.75801084   -
0.00018805   -0.04610803
 1138   16     4.69124    -4.04181    -2.10008     -0.00009083    1.75801084   -
0.00005167   -0.05292446
 1139   16     4.70153    -3.23342    -3.23225     -0.00043553    1.75801084   -
0.00024774   -0.04939481
 1140   16     4.71603    -2.17141    -3.65316      0.00022224    0.87948836
0.00025269   -0.05169337
 1141   18    -0.14547    -3.89510     2.12484      0.00026230    0.87975542
0.00029815   -0.07257287
 1142   18    -0.13689    -3.32593     3.11876     -0.00059842    1.75858876   -
0.00034028   -0.06708201
 1143   18    -0.12129    -2.08668     3.75820     -0.00048816    1.75858876   -
0.00027758   -0.06683449
 1144   17     1.35389    -3.72166     2.51698     -0.00014790    1.75858876   -
0.00008410   -0.06372092
 1145   17     1.36684    -2.78074     3.54624     -0.00047434    1.75858876   -
0.00026973   -0.06018930
 1146   17     1.38022    -1.67270     3.83603      0.00018013    0.87975542
0.00020475   -0.06256667
 1147   25     6.23605    -1.71651     3.82686      0.00018112    0.88005149
0.00020581   -0.04789412
 1148   25     6.22329    -2.82544     3.54329     -0.00046831    1.75916443   -
0.00026621   -0.04558468
 1149   25     6.21144    -3.77156     2.51992     -0.00015554    1.75916443   -
0.00008842   -0.04900434
 1150   17     4.73289    -2.13115     3.75024     -0.00029878    1.75916443   -
0.00016984   -0.04994334
 1151   17     4.71821    -3.37319     3.11802     -0.00041061    1.75916443   -
0.00023341   -0.05040732
 1152   17     4.71056    -3.94762     2.12794      0.00035402    0.88005149
0.00040227   -0.05592049
 1153   27    -4.96816    -3.86934     2.12808     -0.00005011    0.88380768   -
0.00005670   -0.10577080
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 1154   27    -4.95766    -3.30595     3.13561     -0.00101877    1.76677811   -
0.00057662   -0.10183881
 1155   27    -4.94704    -2.06147     3.78759     -0.00088320    1.76677811   -
0.00049989   -0.10297790
 1156   18    -3.47512    -3.68781     2.51665     -0.00053145    1.76677811   -
0.00030080   -0.08975441
 1157   18    -3.46268    -2.74889     3.56173     -0.00079464    1.76677811   -
0.00044977   -0.08713597
 1158   18    -3.45545    -1.63345     3.85905      0.00005613    0.88380768
0.00006351   -0.09030640
 1159   26    -5.05140    -1.92516    -3.64343     -0.00002284    0.84212230   -
0.00002712   -0.10584374
 1160   26    -5.08181    -2.94905    -3.28082     -0.00087028    1.68303624   -
0.00051709   -0.10287761
 1161   26    -5.10784    -3.78819    -2.25324     -0.00071295    1.68303624   -
0.00042361   -0.10457970
 1162   19    -3.54148    -2.36915    -3.52908     -0.00049253    1.68303624   -
0.00029264   -0.08884810
 1163   19    -3.57552    -3.50017    -2.83597     -0.00069268    1.68303624   -
0.00041157   -0.08828573
 1164   19    -3.59149    -3.99751    -1.86996      0.00010360    0.84212230
0.00012302   -0.09247198
 1165   30     8.79016     4.21224     1.68961      0.00035905    0.86006102
0.00041747   -0.04611746
 1166   30     8.78444     3.75006     2.69637     -0.00037158    1.71893151   -
0.00021617   -0.04083059
 1167   30     8.76945     2.62226     3.44054     -0.00042044    1.71893151   -
0.00024459   -0.04057275
 1168   20     7.26594     4.08300     2.08674     -0.00002716    1.71893151   -
0.00001580   -0.04682056
 1169   20     7.25549     3.27150     3.16714     -0.00036184    1.71893151   -
0.00021050   -0.04354209
 1170   20     7.24159     2.23851     3.56709      0.00022777    0.86006102
0.00026483   -0.04580008
 1171   28     8.74405     1.73171    -3.91496      0.00011826    0.85371718
0.00013853   -0.04244458
 1172   28     8.76468     2.79833    -3.65527     -0.00042184    1.70620249   -
0.00024724   -0.04001865
 1173   28     8.78730     3.74010    -2.70239     -0.00010227    1.70620249   -
0.00005994   -0.04325023
 1174   21     7.22516     2.17251    -3.83422     -0.00021240    1.70620249   -
0.00012449   -0.04417042
 1175   21     7.25025     3.37835    -3.25048     -0.00030495    1.70620249   -
0.00017873   -0.04445275
 1176   21     7.26643     3.96851    -2.32474      0.00033551    0.85371718
0.00039300   -0.04947733];
```

[$MDEGSO_4$] (Computation ID = 81)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.30
%   total number of segments         =    941
%   number of charge corr segments   =    424
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% S            -9.44183131798549   -0.50256302344908    0.23190931411137   4.0818
0.0528    28.57     0.00185    6.5385
% O             0.11312462457302   -0.26164855208084   -0.08680979842377   3.2503
0.1276    35.20     0.00363    5.7070
% O            -6.60164014133250    1.17438929779400    0.22440965630487   3.2503
0.1370    37.55     0.00365    5.7070
% O             6.86484613691597    0.95776955177980   -0.07176443018510   3.2503
0.1398    37.84     0.00369    5.7070
% O            -9.44644464779293   -1.82885754195067   -2.25846307363318   3.2503
0.2767    71.29     0.00388    5.7070
% O           -11.24639073685456    1.63004487796435    0.49369429685954   3.2503
0.2859    75.17     0.00380    5.7070
% O            -9.21040531077921   -2.21068877518639    2.46634966767922   3.2503
0.2750    70.78     0.00389    5.7070
% C            -2.14805937311095    1.25305659515752    0.15313467274505   3.7795
0.0007    25.57     0.00003    6.2361
% C             2.33541084174056    1.24601598962130    0.02306744839133   3.7795
0.0015    25.78     0.00006    6.2361
% C            -4.45647001149289   -0.45315889669072    0.01431277433234   3.7795
0.0082    25.87     0.00032    6.2361
% C             4.58992193490799   -0.52287610341666   -0.18724163848668   3.7795
0.0029    25.15     0.00012    6.2361
% C             9.05856394317792   -0.59453032666387   -0.23091785607182   3.7795
0.0124    66.35     0.00019    6.2361
% H            -2.21186892558384    2.67479000439223   -1.37906946313267   2.4566  -
0.0321    25.32    -0.00127    4.9133
% H            -2.12018756816738    2.27437953569561    1.97811945910804   2.4566  -
0.0318    25.20    -0.00126    4.9133
% H             2.43739855001395    2.31212208505786    1.82384837121183   2.4566  -
0.0296    25.17    -0.00118    4.9133
% H             2.37495416026020    2.64460600237171   -1.53607400207417   2.4566  -
0.0296    25.27    -0.00117    4.9133
% H            -4.48628175447432   -1.49305820408546   -1.79584300987438   2.4566  -
0.0229    22.19    -0.00103    4.9133
% H            -4.43137084862471   -1.84433566314115    1.56872987547029   2.4566  -
0.0227    21.56    -0.00105    4.9133
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% H             4.55116774334143   -1.91520858101170    1.37258448243062   2.4566  -
0.0294    25.35    -0.00116    4.9133
% H             4.50244291832295   -1.58104907188872   -1.98948503358339   2.4566  -
0.0294    25.63    -0.00115    4.9133
% H             9.11815762249063   -1.66013364723680   -2.03373394022962   2.4566  -
0.0279    24.32    -0.00115    4.9133
% H             9.14633339555058   -1.96308253605542    1.35264248798221   2.4566  -
0.0280    24.31    -0.00115    4.9133
% H            10.70862876490362    0.66401698302311   -0.13340026093203   2.4566  -
0.0391    24.16    -0.00162    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =      -1047.076642
%   Total energy + OC corr.      =      -1047.081511
%   Dielectric energy            =         -0.107965      -2.938      -67.75
%   Diel. energy + OC corr.      =         -0.112834      -3.070      -70.81
%
%   Surface area of cavity [au]
acosmo =           793.594;
%   Total Volume of cavity [au]
vcosmo =          1439.758;
%
%
% $screening_charge
%   cosmo           =    0.95707
%   corrected total =    0.99812
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1   -11.65572    -3.92187    -0.02891      0.00119394    0.58050918
0.00205672   -0.21069309
    2    1    -9.14458     2.12127    -2.88071      0.00069183    0.58050918
0.00119176   -0.21030640
    3    1   -13.04011    -1.79443     1.66175      0.00054289    0.77401224
0.00070139   -0.20446308
    4    1    -9.08143     1.71014     3.64296      0.00113734    0.96751531
0.00117553   -0.21163196
    5    1    -9.83650     1.92396    -3.02653      0.00079793    0.58050918
0.00137454   -0.21608772
    6    1   -13.15348    -1.32392    -1.25470      0.00092327    1.35452143
0.00068162   -0.20775508
    7    1   -13.36743    -1.57825     0.53778      0.00063673    1.16101837
0.00054842   -0.19918855
    8    1   -12.78438    -1.24129     2.45512      0.00129602    0.38700612
0.00334884   -0.21640945
    9    1    -8.47406     1.18144     3.82200      0.00042547    0.19350306
0.00219879   -0.21005145
   10    1    -8.68198     1.94515    -2.94498      0.00077481    0.38700612
0.00200206   -0.20923977
   11    1   -12.42985    -3.27736     0.04958      0.00043453    1.35452143
0.00032080   -0.19918115
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0.00004679   -0.19590114
   13    1    -8.48624     1.58347     3.60779      0.00027735    0.19350306
0.00143332   -0.20941338
   14    1   -13.06597    -2.25241    -0.44972     -0.00021343    1.74152755   -
0.00012255   -0.19613881
   15    2     0.11861    -2.76963     1.98071      0.00416940    0.73618757
0.00566350   -0.13997226
   16    2     0.31836    -3.15775    -1.54796      0.00494570    0.98158343
0.00503849   -0.13858239
   17    2    -0.31885    -3.21897     1.19079      0.00250391    0.49079171
0.00510178   -0.14352781
   18    2    -0.42708    -3.32965    -1.01419      0.00266513    0.61348964
0.00434421   -0.14324831
   19    2     0.13800    -3.41359     0.70641      0.00280675    0.61348964
0.00457506   -0.14089443
   20    2     0.33006    -3.46101    -0.61739      0.00320306    0.85888550
0.00372933   -0.13844627
   21    2    -0.04382    -2.75807    -2.16232      0.00514489    0.98158343
0.00524142   -0.14123627
   22    2    -0.44814    -1.70682    -2.94355      0.00215270    0.49079171
0.00438618   -0.14004064
   23    2    -0.15828    -2.23626     2.48066      0.00265327    0.49079171
0.00540611   -0.13888659
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0.00524270   -0.13921432
   25    2     0.18705    -1.18964    -3.20095      0.00348081    0.61348964
0.00567379   -0.13272406
   26    2    -0.04080    -0.47673    -3.32634      0.00425508    0.98158343
0.00433491   -0.12726241
   27    2     0.46630    -1.54255     2.87955      0.00198567    0.36809379
0.00539448   -0.12913855
   28    2     0.30174    -2.08768     2.59548      0.00239904    0.49079171
0.00488811   -0.13498292
   29    2    -0.36024    -3.47021     0.12675      0.00260783    0.61348964
0.00425081   -0.14331173
   30    2     0.56941    -3.45753     0.29093      0.00276003    0.61348964
0.00449891   -0.13630499
   31    2     0.11578    -2.06415    -2.79152      0.00480107    0.85888550
0.00558989   -0.13833704
   32    2    -0.05350    -1.23211     3.01080      0.00390979    0.85888550
0.00455217   -0.12881809
   33    3    -6.64263     3.58826    -1.95185      0.00348476    0.73618757
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   34    3    -6.16877     4.12999     1.50568      0.00505561    1.22697929
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   35    3    -7.00782     2.22784     3.27236      0.00249168    0.61348964
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   36    3    -7.35351     3.95064    -1.28943      0.00340794    0.85888550
0.00396786   -0.20180588
   37    3    -7.14969     4.26230     1.07827      0.00406861    1.10428136
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   38    3    -6.67105     4.26768    -0.77123      0.00285238    0.73618757
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   42    3    -7.48017     3.29410    -2.07768      0.00361740    0.73618757
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   43    3    -6.33908     4.00165    -1.35743      0.00296150    0.61348964
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   44    3    -6.07328     2.14602     3.28079      0.00175101    0.36809379
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   45    3    -6.40162     1.60090     3.44043      0.00318108    0.61348964
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   46    3    -6.37257     2.24509    -2.83593      0.00305063    0.61348964
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   59    4     6.66206     2.36418     2.85149      0.00400528    0.85888550
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  121    6   -13.68801     3.37288     1.74493      0.00400413    1.47237514
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  144    6   -12.26494     2.16191    -2.54675      0.00551365    1.10428136
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  148    6   -10.83488     2.63455     3.55740      0.00584561    1.22697929
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  149    6   -12.80881     0.95821     3.26354      0.00528024    1.10428136
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  150    6   -14.33017     2.29155     1.27935      0.00459259    1.47237514
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  158    6    -9.88763     4.17233     1.99546      0.00310066    0.73618757
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  160    7    -8.93167    -4.10161     5.09530      0.00349720    1.34967722
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0.00020070   -0.13119101
  799   14    -3.50216     1.50564     3.82524     -0.00179817    1.03939331   -
0.00173001   -0.11049471
  800   10    -4.03896     0.53337     3.69151     -0.00047195    1.46388274   -
0.00032240   -0.12850199
  801   17    -4.95720    -0.20486    -3.83421     -0.00031894    0.24701184   -
0.00129120   -0.13596292
  802   17    -4.08300    -0.20482    -3.84864     -0.00021491    0.24701184   -
0.00087002   -0.12128449
  803   10    -4.51724     0.16400    -3.66683     -0.00079345    0.53775078   -
0.00147550   -0.12914320
  804   17    -3.09959    -3.50151    -1.97095     -0.00042885    0.29201225   -
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  805   17    -4.34299    -3.85872    -1.74525     -0.00108758    0.67657944   -
0.00160747   -0.12923952
  806   10    -3.45685    -3.70076    -1.46406     -0.00086884    0.61248204   -
0.00141855   -0.12359102
  807   10    -4.86260    -3.97318    -1.28439     -0.00013740    0.35395425   -
0.00038819   -0.14263538
  808   18    -4.13666    -1.02619     3.81856     -0.00071583    0.41101246   -
0.00174163   -0.12521654
  809   10    -4.37727    -0.59950     3.75532     -0.00063605    0.49819692   -
0.00127671   -0.13183727
  810   18    -4.83152    -4.18844     0.99963     -0.00039596    0.29874343   -
0.00132542   -0.14003457
  811   18    -3.51451    -3.98573     1.15981     -0.00121804    0.69747728   -
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0.00093327   -0.12262035
  814   11     6.24245    -0.92891     3.22436     -0.00008229    0.21040801   -
0.00039109   -0.06110282
  815   12     6.98350    -0.93977     3.14395      0.00001070    0.21040801
0.00005087   -0.06034779
  816   19     6.12498    -1.20312     3.26982     -0.00029541    0.21040801   -
0.00140400   -0.05656183
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0.00066872   -0.05024512
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0.00042810   -0.04769185
  819   19     6.05763    -3.92292     0.84031     -0.00030095    0.21040801   -
0.00143031   -0.04913224
  820   11     6.14848    -3.68772    -1.63127     -0.00010164    0.20885855   -
0.00048665   -0.05019455
  821   12     6.89148    -3.62975    -1.61448     -0.00015928    0.20885855   -
0.00076262   -0.04695017
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0.00153029   -0.04871621
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0.00035709   -0.06109354
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0.00163084   -0.05628746
  826   12     7.33323     0.09992    -3.65770     0.00045977    0.54433293
0.00084464   -0.06530455
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0.00089783   -0.07025045
  828   12     7.39272    -0.42227     3.28847     0.00051185    0.57656429
0.00088775   -0.06740275
  829   11     6.32680    -0.53593     3.30186     0.00039345    0.57656429
0.00068240   -0.06793832
  830   12     7.30053    -3.94715    -0.36265    -0.00020480    1.75703375   -
0.00011656   -0.04804191
  831   11     6.23349    -3.88992    -0.74386    -0.00046879    1.75703375   -
0.00026681   -0.05246089
  832   15     3.66185     1.32906     3.68231    -0.00176123    1.02843552   -
0.00171254   -0.06428794
  833   11     4.56953     0.72779     3.43404    -0.00022765    1.44860602   -
0.00015715   -0.07204072
  834   16     3.76210     2.24435    -3.49404    -0.00169645    1.03372078   -
0.00164111   -0.06457358
  835   11     4.26646     1.24887    -3.56852    -0.00038361    1.45593199   -
0.00026348   -0.07020642
  836   19     5.42389    -1.20959     3.53672    -0.00049467    0.32910620   -
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  837   19     4.28806    -1.06138     3.64079    -0.00045856    0.32910620   -
0.00139334   -0.06019387
  838   11     4.89427    -0.76082     3.47311    -0.00135003    0.67053407   -
0.00201337   -0.05939276
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0.00120075   -0.07349681
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0.00141504   -0.06002800
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  843   11     5.02541    -4.16916     0.43390    -0.00064606    0.56575546   -
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  844   20     4.18139    -0.29904    -4.03528    -0.00048750    0.33777685   -
0.00144326   -0.06025409
  845   20     5.34579    -0.47470    -3.98866    -0.00060169    0.33777685   -
0.00178134   -0.05545177
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0.00026712   -0.05535537
  856   19     6.55694    -1.36792     3.19364     -0.00023103    0.28492840   -
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  857   22     7.54024    -1.36597     3.26451     -0.00041163    0.28492840   -
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  858   12     7.33130    -0.94954     3.33793      0.00002296    0.00588925
0.00389896   -0.05909755
  859   19     5.99508    -4.02891     1.03123      0.00005938    0.08498105
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  860   12     7.27407    -4.04793     0.62505      0.00015405    0.12054600
0.00127795   -0.04691547
  861   12     7.37194    -0.46703    -3.67765     -0.00025226    0.28634999   -
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  865   20     6.47022    -3.52495    -2.05569     -0.00014587    0.28634999   -
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  868   12     7.27756    -0.28752    -3.77943      0.00006397    0.04917643
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  871   21     8.16309    -0.56914    -4.01580     -0.00034374    0.25507534   -
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  874   21    11.24159    -1.91492    -3.11856     -0.00074838    0.56919925   -
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  892   12     8.52417    -4.21683     0.47919     -0.00039196    0.55238166   -
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  895   12    11.51710    -2.13296     2.11425     -0.00046126    0.55238166   -
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  896   12    10.78374    -1.11500     3.03464     -0.00029274    0.55238166   -
0.00052996   -0.04011710
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  899   23    10.41144     2.86156     0.92692     -0.00040333    0.23718515   -
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  901   23    11.61557     1.19728     2.03103     -0.00088593    0.52423491   -
0.00168994   -0.03541924
  902   23    12.37906     0.23393     1.54480     -0.00093607    0.52423491   -
0.00178559   -0.02915741
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0.00197777   -0.02453729
  904   23    12.83366    -0.17334    -0.89150     -0.00102505    0.52423491   -
0.00195533   -0.02457894
  905   23    12.34748     0.54156    -1.89147     -0.00086589    0.52423491   -
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  906   23    11.57682     1.57470    -2.18487     -0.00084233    0.52423491   -
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  919   16     0.73189     3.70989    -3.22335     -0.00209003    1.81194113   -
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  925   15     0.89791     3.63367     3.41965     -0.00206748    1.81184730   -
0.00114109   -0.06511554
  926   15     0.92641     2.21623     3.91449     -0.00203666    1.81184730   -
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  927   14    -0.52260     4.09622     2.86789     -0.00194558    1.81184730   -
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0.00088770   -0.03927353
  933   19     6.14988    -2.23907     3.37951     -0.00196576    1.80528954   -
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  934   19     6.13325    -3.52647     2.63332     -0.00195579    1.80528954   -
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  939   20     6.06258    -3.41545    -2.93881     -0.00167042    1.80816521   -
0.00092382   -0.04548390
  940   20     6.07231    -2.29951    -3.91811     -0.00199458    1.80816521   -
0.00110309   -0.04480794
  941   20     6.09181    -1.08367    -4.05684     -0.00041173    0.90401036   -
0.00045545   -0.05187597];
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[$MESO_3$] (Computation ID = 845)

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% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.30
%   total number of segments         =    381
%   number of charge corr segments   =    216
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% S             0.00000000000000    0.00000000000000    1.71136971115405   4.0818
0.0653    25.95     0.00252    6.5385
% O             1.37777758030658   -2.38638077062031    2.39794404795396   3.2503
0.3403    75.38     0.00452    5.7070
% O            -2.75555516061316    0.00000000000000    2.39794404795396   3.2503
0.3400    75.87     0.00448    5.7070
% C             0.00000000000000    0.00000000000000   -1.73733506810164   3.7795
0.0259    53.70     0.00048    6.2361
% O             1.37777758030658    2.38638077062031    2.39794404795396   3.2503
0.3392    75.35     0.00450    5.7070
% H            -0.98613818700974    1.70804144318473   -2.38928892897143   2.4566  -
0.0373    25.57    -0.00146    4.9133
% H            -0.98613818700974   -1.70804144318473   -2.38928892897143   2.4566  -
0.0379    25.50    -0.00149    4.9133
% H             1.97227637401949    0.00000000000000   -2.38928892897143   2.4566  -
0.0373    25.57    -0.00146    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -664.082633
%   Total energy + OC corr.      =       -664.087910
%   Dielectric energy            =         -0.110645      -3.011      -69.43
%   Diel. energy + OC corr.      =         -0.115922      -3.154      -72.74
%
%   Surface area of cavity [au]
acosmo =           382.879;
%   Total Volume of cavity [au]
vcosmo =           623.635;
%
%
% $screening_charge
%   cosmo           =    0.97065
%   corrected total =    0.99816
%
%
% $segment information
```

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%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1    -2.02994     3.44762     0.90239      0.00144586    0.77401224
0.00186801   -0.20774667
    2    1    -0.70915    -0.87516     5.63467      0.00108081    0.96751531
0.00111710   -0.22863911
    3    1    -1.12324     1.98633     5.09575      0.00189156    0.38700612
0.00488767   -0.24275925
    4    1     4.00014    -0.05592     0.90080      0.00097722    0.38700612
0.00252507   -0.20834599
    5    1     1.58297    -0.05739     5.47330      0.00083853    0.58050918
0.00144448   -0.23371472
    6    1     0.39613    -0.48597     5.74474      0.00144364    1.35452143
0.00106580   -0.22462915
    7    1    -0.97718    -1.66432     5.30806      0.00145903    0.58050918
0.00251337   -0.23779109
    8    1    -1.94977    -3.48228     0.85515      0.00050100    0.19350306
0.00258913   -0.20694600
    9    1    -0.62254     1.15335     5.57704      0.00103757    1.35452143
0.00076600   -0.23008928
   10    1    -0.55695     0.18764     5.75064      0.00118823    1.16101837
0.00102344   -0.22426098
   11    1     0.71609     0.43126     5.70667      0.00152155    1.16101837
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   12    2     3.02987    -5.08695     3.13423      0.00419709    1.34967722
0.00310970   -0.20458564
   13    2     4.18061    -2.03798     4.00649      0.00570710    1.22697929
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   14    2     4.13474    -2.99255     0.78664      0.00600385    1.22697929
0.00489319   -0.21044854
   15    2     1.50207    -4.83118     0.25972      0.00567213    0.98158343
0.00577855   -0.20518350
   16    2    -0.35150    -5.04555     3.10718      0.00570572    1.22697929
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   17    2     1.27090    -3.25706     5.52767      0.00486541    0.98158343
0.00495670   -0.23357707
   18    2     3.67127    -4.26127     3.73559      0.00497864    1.47237514
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   19    2     4.13546    -3.21239     3.90710      0.00502377    1.22697929
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   20    2     3.77025    -4.58596     2.34808      0.00491543    1.47237514
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  316    4    -3.82712     0.76176    -1.53171      0.00184013    1.35008413
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  317    3    -4.35676     0.00000    -0.39971      0.01122502    2.46027014
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  318    5    -1.59143     4.00605     2.54388      0.00524112    1.11311359
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  319    5    -1.25335     3.42050     4.07738      0.01067612    2.23093549
0.00478549   -0.24598800
  320    3    -2.56611     3.19504     3.15201      0.01060796    2.23093549
0.00475494   -0.24217046
  321    3    -2.15752     2.48735     4.61523      0.00502696    1.11311359
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  322    6    -3.43874     2.13567    -1.57603     -0.00032463    1.14327968   -
0.00028394   -0.14298238
  323    6    -2.80456     3.01258    -1.02874     -0.00055707    1.14327968   -
0.00048726   -0.14842307
  324    3    -3.75159     2.18937     0.04409      0.01012497    2.85649555
0.00354454   -0.19908814
  325    7    -2.80454    -3.01259    -1.02872     -0.00062309    1.14330746   -
0.00054499   -0.14836555
  326    7    -3.43875    -2.13566    -1.57601     -0.00035892    1.14330746   -
0.00031393   -0.14294509
  327    3    -3.75158    -2.18937     0.04410      0.01034629    2.85656129
0.00362194   -0.19906866
  328    4     0.60642     3.76043    -1.50217      0.00031177    0.21789207
0.00143083   -0.15441846
  329    5     0.82817     4.00442    -0.70175      0.00132971    0.21789207
0.00610262   -0.18518969
  330    6     0.34101     3.81051    -1.62824     -0.00009830    0.21789207   -
0.00045113   -0.14676419
  331    4     2.95347     2.40533    -1.50216      0.00032261    0.21788452
0.00148065   -0.15455482
  332    5     3.05390     2.71936    -0.70174      0.00124479    0.21788452
0.00571306   -0.18480650
  333    8     3.12954     2.20050    -1.62823     -0.00007553    0.21788452   -
0.00034663   -0.14694097
  334    5     2.83682     3.44058    -0.42727      0.00575642    1.21534875
0.00473643   -0.19600560
  335    5     1.56131     4.17701    -0.42728      0.00539548    1.21534875
0.00443945   -0.19598205
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  336    4     1.88974     3.27304    -1.49996      0.00379161    2.68545953
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  339    6    -0.17768     2.81165    -4.36993     -0.00072106    0.52171368   -
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  340    6    -1.19760     2.07432    -4.75900     -0.00077474    0.52171368   -
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  341    6    -2.34613     1.55977    -4.36990     -0.00069140    0.52171368   -
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0.00140029   -0.12680527
  344    4     0.67418     3.56848    -2.62034     -0.00049000    0.51690963   -
0.00094795   -0.12566607
  345    4     0.51094     2.96499    -3.95457     -0.00041967    0.51690963   -
0.00081188   -0.10668535
  346    4    -0.38143     2.13408    -4.78178     -0.00047318    0.51690963   -
0.00091540   -0.09815719
  347    4    -1.65748     1.39739    -4.78176     -0.00051678    0.51690963   -
0.00099976   -0.09810054
  348    4    -2.82325     1.04011    -3.95452     -0.00043135    0.51690963   -
0.00083449   -0.10687304
  349    4    -3.42748     1.20053    -2.62028     -0.00056650    0.51690963   -
0.00109594   -0.12566936
  350    7    -3.44351    -1.70633    -2.32600     -0.00038204    0.23620836   -
0.00161739   -0.12677546
  351    7    -3.17867    -1.46716    -3.35323     -0.00079067    0.52169522   -
0.00151558   -0.10938258
  352    7    -2.34614    -1.55978    -4.36988     -0.00079730    0.52169522   -
0.00152829   -0.09770922
  353    7    -1.19763    -2.07437    -4.75897     -0.00075902    0.52169522   -
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  354    7    -0.17775    -2.81173    -4.36987     -0.00082652    0.52169522   -
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  355    7     0.31870    -3.48641    -3.35320     -0.00075486    0.52169522   -
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  356    7     0.24398    -3.83534    -2.32598     -0.00032984    0.23620836   -
0.00139641   -0.12643259
  357    4    -3.42749    -1.20053    -2.62028     -0.00051797    0.51688263   -
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  358    4    -2.82326    -1.04012    -3.95451     -0.00038835    0.51688263   -
0.00075134   -0.10684649
  359    4    -1.65749    -1.39745    -4.78174     -0.00047851    0.51688263   -
0.00092576   -0.09813238
  360    4    -0.38147    -2.13417    -4.78173     -0.00048795    0.51688263   -
0.00094403   -0.09815539
  361    4     0.51084    -2.96510    -3.95449     -0.00048866    0.51688263   -
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  362    4     0.67401    -3.56857    -2.62025     -0.00049143    0.51688263   -
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  363    8     3.19947    -2.12900    -2.32600     -0.00033237    0.23621256   -
0.00140708   -0.12654427
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  364    8     2.85992    -2.01924    -3.35322     -0.00079850    0.52170212   -
0.00153056   -0.10946662
  365    8     2.52386    -1.25195    -4.36988     -0.00068309    0.52170212   -
0.00130935   -0.09784904
  366    8     2.39523    -0.00003    -4.75899     -0.00079111    0.52170212   -
0.00151641   -0.09391138
  367    8     2.52383     1.25190    -4.36991     -0.00066087    0.52170212   -
0.00126676   -0.09787507
  368    8     2.85988     2.01922    -3.35327     -0.00071983    0.52170212   -
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  369    8     3.19943     2.12901    -2.32605     -0.00035755    0.23621256   -
0.00151369   -0.12654556
  370    4     2.75341    -2.36804    -2.62027     -0.00053279    0.51689444   -
0.00103075   -0.12561590
  371    4     2.31238    -1.92498    -3.95450     -0.00045212    0.51689444   -
0.00087469   -0.10672803
  372    4     2.03893    -0.73675    -4.78174     -0.00044871    0.51689444   -
0.00086808   -0.09827983
  373    4     2.03892     0.73668    -4.78176     -0.00045155    0.51689444   -
0.00087359   -0.09825548
  374    4     2.31234     1.92493    -3.95455     -0.00050606    0.51689444   -
0.00097904   -0.10680192
  375    4     2.75337     2.36803    -2.62032     -0.00051078    0.51689444   -
0.00098817   -0.12560429
  376    6    -1.20665     3.93513    -1.02876     -0.00073327    1.14335735   -
0.00064133   -0.14841159
  377    6    -0.13005     4.04587    -1.57607     -0.00038448    1.14335735   -
0.00033627   -0.14294247
  378    5    -0.02017     4.34364     0.04405      0.01025185    2.85668370
0.00358872   -0.19892907
  379    8     3.56888     1.91024    -1.57606     -0.00029435    1.14330830   -
0.00025745   -0.14296184
  380    8     4.01124     0.92254    -1.02877     -0.00055659    1.14330830   -
0.00048682   -0.14841222
  381    5     3.77182     2.15430     0.04405      0.01015789    2.85656141
0.00355599   -0.19896941];
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[TCB] (Computation ID = 850)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.26
%   total number of segments         =    516
%   number of charge corr segments   =    320
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N            -3.86052218711210    3.86052218711210    0.00000000000000   3.4582
0.2507    94.91     0.00264    5.9148
% N             3.86052218711210   -3.86052218711210    0.00000000000000   3.4582
0.2504    94.79     0.00264    5.9148
% N            -3.86052218711210   -3.86052218711210    0.00000000000000   3.4582
0.2505    94.93     0.00264    5.9148
% N             3.86052218711210    3.86052218711210    0.00000000000000   3.4582
0.2509    95.04     0.00264    5.9148
% C            -2.27791065361089    2.27791065361089    0.00000000000000   3.7795
0.0194    44.19     0.00044    6.2361
% C             2.27791065361089   -2.27791065361089    0.00000000000000   3.7795
0.0197    44.44     0.00044    6.2361
% C            -2.27791065361089   -2.27791065361089    0.00000000000000   3.7795
0.0192    44.19     0.00044    6.2361
% C             2.27791065361089    2.27791065361089    0.00000000000000   3.7795
0.0187    43.94     0.00042    6.2361
% B             0.00000000000000    0.00000000000000    0.00000000000000   3.8692  -
0.0805    22.81    -0.00353    6.3259
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                  =       -396.397731
%   Total energy + OC corr.       =       -396.402730
%   Dielectric energy             =         -0.075898      -2.065      -47.63
%   Diel. energy + OC corr.       =         -0.080898      -2.201      -50.77
%
%   Surface area of cavity [au]
acosmo =           579.240;
%   Total Volume of cavity [au]
vcosmo =          1027.246;
%
%
% $screening_charge
%   cosmo           =    0.96571
%   corrected total =    0.99904
%
```

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%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1    -6.23416     6.37542     0.01675      0.00576289    1.52783059
0.00377194   -0.16187492
    2    1    -3.52689     6.38490    -2.33997      0.00354116    1.38893690
0.00254955   -0.15422380
    3    1    -2.92229     6.99158     1.12935      0.00372579    1.38893690
0.00268247   -0.15753198
    4    1    -5.13566     4.90250     3.04096      0.00307287    1.25004321
0.00245821   -0.15159794
    5    1    -7.10029     2.97871     0.82783      0.00376175    1.38893690
0.00270837   -0.15796320
    6    1    -6.14088     3.74167    -2.59710      0.00283091    1.11114952
0.00254773   -0.15338974
    7    1    -5.58100     6.67158    -1.04742      0.00582334    1.66672428
0.00349388   -0.16023076
    8    1    -4.57150     6.75610    -1.75195      0.00425537    1.38893690
0.00306376   -0.15728248
    9    1    -5.20868     7.02190     0.38380      0.00589266    1.66672428
0.00353547   -0.16074096
   10    1    -4.04348     7.23940     0.71341      0.00441346    1.38893690
0.00317758   -0.15890704
   11    1    -6.11814     6.14629     1.27966      0.00580425    1.66672428
0.00348243   -0.15994635
   12    1    -5.87298     5.47485     2.30284      0.00450301    1.52783059
0.00294732   -0.15585719
   13    1    -6.93736     5.39028     0.38989      0.00555953    1.52783059
0.00363884   -0.16103773
   14    1    -7.25391     4.23181     0.55324      0.00445924    1.38893690
0.00321054   -0.15929694
   15    1    -6.67918     5.61589    -0.96588      0.00683328    1.94451166
0.00351414   -0.16032816
   16    1    -6.58749     4.76140    -1.92644      0.00497984    1.66672428
0.00298780   -0.15679181
   17    1    -3.25120     6.99802    -1.32064      0.00378444    1.38893690
0.00272470   -0.15721138
   18    1    -3.02997     7.21557    -0.11455      0.00421199    1.52783059
0.00275685   -0.15842736
   19    1    -3.62086     6.70014     1.95917      0.00440406    1.66672428
0.00264234   -0.15554421
   20    1    -4.43041     5.86943     2.75657      0.00412798    1.66672428
0.00247671   -0.15284220
   21    1    -6.05611     4.14112     2.65702      0.00409818    1.66672428
0.00245883   -0.15309270
   22    1    -6.77781     3.51128     1.82386      0.00444242    1.66672428
0.00266536   -0.15591231
   23    1    -7.20321     3.03785    -0.32961      0.00420331    1.52783059
0.00275116   -0.15837646
   24    1    -6.84773     3.36799    -1.67124      0.00437375    1.66672428
0.00262416   -0.15624683
   25    1    -5.59094     4.78807    -2.84683      0.00378444    1.52783059
0.00247700   -0.15262223
   26    1    -4.56868     5.80486    -2.77078      0.00447007    1.80561797
0.00247565   -0.15279015
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   27    1    -2.50109     6.43444    -1.86713      0.00251351    0.97225583
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   28    1    -1.79943     6.17372    -1.53632      0.00180574    0.55557476
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   29    1    -1.96468     6.69802     0.56006      0.00332945    1.25004321
0.00266347   -0.15891298
   30    1    -2.11075     6.25807     1.77463      0.00436406    1.66672428
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   31    1    -2.43745     5.60722     2.62357      0.00142925    0.69446845
0.00205804   -0.15267301
   32    1    -3.23416     4.79621     3.26976      0.00261851    0.97225583
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   33    1    -4.12083     4.80023     3.31788      0.00242798    1.11114952
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   34    1    -5.02863     3.79710     3.25432      0.00262458    1.11114952
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   35    1    -5.23273     2.85701     3.01148      0.00242908    0.97225583
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   36    1    -6.06578     1.95427     1.86065      0.00204839    0.69446845
0.00294958   -0.15607881
   37    1    -6.54097     2.18094     1.39756      0.00274212    1.11114952
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   38    1    -6.72101     1.92490     0.17304      0.00434605    1.52783059
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   39    1    -6.11273     2.08195    -1.92958      0.00285065    0.97225583
0.00293200   -0.15585491
   40    1    -6.05344     2.79597    -2.45293      0.00224067    0.97225583
0.00230461   -0.15363640
   41    1    -5.23580     3.77449    -3.17180      0.00259965    1.11114952
0.00233961   -0.15018798
   42    1    -4.36423     3.77554    -3.42026      0.00210270    0.97225583
0.00216270   -0.14786704
   43    1    -3.41262     4.46150    -3.37600      0.00208401    0.83336214
0.00250072   -0.14784267
   44    1    -3.23237     5.35304    -3.05566      0.00301682    1.25004321
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   45    1    -4.34213     7.22985    -0.61228      0.00528978    1.66672428
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   46    1    -5.00070     6.61978     1.74519      0.00603056    1.94451166
0.00310132   -0.15758904
   47    1    -6.77992     4.81497     1.58909      0.00522626    1.66672428
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   48    1    -7.21913     4.27708    -0.71080      0.00570009    1.80561797
0.00315686   -0.15900676
   49    1    -5.69792     5.87312    -2.12899      0.00511695    1.66672428
0.00307006   -0.15669725
   50    1    -2.03916     6.71282    -0.71157      0.00389258    1.52783059
0.00254778   -0.15859011
   51    1    -3.24384     5.85238     2.75888      0.00295888    1.25004321
0.00236702   -0.15225064
   52    1    -5.95116     2.69919     2.49791      0.00305982    1.38893690
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   53    1    -6.66205     2.17406    -1.12528      0.00352938    1.38893690
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   54    1    -4.31248     4.79389    -3.29905      0.00240529    1.11114952
0.00216469   -0.14958841
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   55    1    -4.17665     3.73601     3.44146      0.00149338    0.83336214
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   57    1    -2.42661     5.71359    -2.54348      0.00222564    1.11114952
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   59    2     6.38492    -3.52685     2.33994      0.00354354    1.38893690
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   60    2     6.99157    -2.92237    -1.12940      0.00372750    1.38893690
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   61    2     4.90243    -5.13578    -3.04091      0.00307661    1.25004321
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   62    2     2.97864    -7.10031    -0.82770      0.00376009    1.38893690
0.00270717   -0.15796759
   63    2     3.74165    -6.14079     2.59719      0.00282971    1.11114952
0.00254666   -0.15338417
   64    2     6.67155    -5.58100     1.04746      0.00582300    1.66672428
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   65    2     6.75610    -4.57149     1.75196      0.00425445    1.38893690
0.00306310   -0.15727898
   66    2     7.02187    -5.20874    -0.38377      0.00589058    1.66672428
0.00353423   -0.16073868
   67    2     7.23937    -4.04355    -0.71343      0.00441394    1.38893690
0.00317792   -0.15890787
   68    2     6.14623    -6.11822    -1.27960      0.00580703    1.66672428
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   69    2     5.47478    -5.87308    -2.30278      0.00449940    1.52783059
0.00294496   -0.15585119
   70    2     5.39022    -6.93739    -0.38979      0.00556270    1.52783059
0.00364091   -0.16104155
   71    2     4.23174    -7.25394    -0.55312      0.00445733    1.38893690
0.00320916   -0.15929695
   72    2     5.61585    -6.67918     0.96596      0.00683536    1.94451166
0.00351521   -0.16033101
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  398    6     1.26405    -5.24923    -2.07758      0.00121857    0.57751843
0.00211000   -0.15058742
  399    2     5.17194    -2.09570    -2.47947      0.00275255    1.16772207
0.00235719   -0.15265863
  400    2     3.63384    -3.63380    -3.29838      0.00246580    1.16772207
0.00211164   -0.14709134
  401    2     2.09572    -5.17189    -2.47949      0.00275433    1.16772207
0.00235872   -0.15254990
  402    3    -5.52743    -1.04440    -1.54230      0.00036923    0.11240326
0.00328485   -0.15395575
  403    5    -5.25151     0.02773    -1.54387      0.00022489    0.11240326
0.00200072   -0.14756337
  404    7    -5.34528    -0.72300    -1.59874      0.00018083    0.11240326
0.00160872   -0.15028688
  405    3    -1.04440    -5.52742    -1.54230      0.00038355    0.11240606
0.00341223   -0.15397075
  406    6     0.02774    -5.25149    -1.54386      0.00022005    0.11240606
0.00195760   -0.14757202
  407    7    -0.72301    -5.34526    -1.59873      0.00022987    0.11240606
0.00204496   -0.15030945
  408    7    -1.26404    -5.24922    -2.07759      0.00129972    0.57752253
0.00225051   -0.15063146
  409    7    -2.41641    -4.09685    -3.15633      0.00219208    1.15156703
0.00190356   -0.14324045
  410    7    -4.09686    -2.41640    -3.15633      0.00221852    1.15156703
0.00192652   -0.14321848
  411    7    -5.24924    -1.26404    -2.07760      0.00117137    0.57752253
0.00202826   -0.15057539
  412    3    -2.09571    -5.17188    -2.47949      0.00274903    1.16772634
0.00235417   -0.15263641
  413    3    -3.63380    -3.63379    -3.29838      0.00246980    1.16772634
0.00211505   -0.14708022
  414    3    -5.17190    -2.09571    -2.47950      0.00275223    1.16772634
0.00235692   -0.15252947
  415    7    -5.24927    -1.26402     2.07757      0.00133633    0.57752913
0.00231388   -0.15054837
  416    7    -4.09690    -2.41639     3.15634      0.00214988    1.15158097
0.00186690   -0.14330361
  417    7    -2.41643    -4.09686     3.15636      0.00219704    1.15158097
0.00190785   -0.14326728
  418    7    -1.26404    -5.24923     2.07761      0.00131883    0.57752913
0.00228358   -0.15054067
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  419    3    -5.17193    -2.09569     2.47949      0.00272291    1.16774184
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  420    3    -3.63383    -3.63379     3.29840      0.00252126    1.16774184
0.00215909   -0.14708431
  421    3    -2.09572    -5.17189     2.47951      0.00266292    1.16774184
0.00228041   -0.15258401
  422    4     1.04440     5.52741    -1.54234      0.00038702    0.11240138
0.00344319   -0.15395869
  423    5    -0.02773     5.25149    -1.54390      0.00022058    0.11240138
0.00196245   -0.14756232
  424    8     0.72301     5.34526    -1.59877      0.00023515    0.11240138
0.00209203   -0.15027949
  425    4     5.52739     1.04441     1.54238      0.00038348    0.11241413
0.00341135   -0.15398249
  426    6     5.25148    -0.02771     1.54394      0.00021853    0.11241413
0.00194400   -0.14758066
  427    8     5.34524     0.72302     1.59882      0.00022952    0.11241413
0.00204175   -0.15032427
  428    4     5.52735     1.04442    -1.54246      0.00037408    0.11241413
0.00332765   -0.15398058
  429    6     5.25143    -0.02771    -1.54402      0.00022189    0.11241413
0.00197383   -0.14758267
  430    8     5.34519     0.72303    -1.59890      0.00018162    0.11241413
0.00161567   -0.15029371
  431    8     5.24919     1.26407     2.07767      0.00129642    0.57751149
0.00224484   -0.15065514
  432    8     4.09683     2.41646     3.15637      0.00218935    1.15154444
0.00190123   -0.14323131
  433    8     2.41640     4.09691     3.15633      0.00221812    1.15154444
0.00192621   -0.14321361
  434    8     1.26404     5.24927     2.07758      0.00118893    0.57751149
0.00205871   -0.15056533
  435    4     5.17185     2.09574     2.47955      0.00274691    1.16770430
0.00235240   -0.15263304
  436    4     3.63377     3.63385     3.29839      0.00246836    1.16770430
0.00211386   -0.14707525
  437    4     2.09570     5.17192     2.47948      0.00275275    1.16770430
0.00235741   -0.15252530
  438    8     1.26403     5.24922    -2.07762      0.00131473    0.57750057
0.00227658   -0.15054727
  439    8     2.41636     4.09687    -3.15634      0.00214818    1.15152138
0.00186551   -0.14329243
  440    8     4.09676     2.41644    -3.15639      0.00219348    1.15152138
0.00190485   -0.14326099
  441    8     5.24913     1.26407    -2.07774      0.00130024    0.57750057
0.00225149   -0.15054111
  442    4     2.09569     5.17188    -2.47952      0.00271986    1.16767865
0.00232928   -0.15256149
  443    4     3.63372     3.63382    -3.29841      0.00251910    1.16767865
0.00215736   -0.14707843
  444    4     5.17179     2.09574    -2.47961      0.00265900    1.16767865
0.00227717   -0.15257951
  445    5    -2.23596     0.38105    -3.39032     -0.00089094    0.28319425   -
0.00314604   -0.10219856
  446    7    -2.23597    -0.38110    -3.39031     -0.00097112    0.28319425   -
0.00342918   -0.10218873
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  447    9    -1.86881    -0.00003    -3.43263     -0.00133313    0.28319425   -
0.00470749   -0.09510005
  448    5    -2.23593     0.38110     3.39031     -0.00097432    0.28319425   -
0.00344046   -0.10219772
  449    7    -2.23593    -0.38104     3.39032     -0.00089613    0.28319425   -
0.00316437   -0.10220337
  450    9    -1.86877     0.00003     3.43263     -0.00135307    0.28319425   -
0.00477787   -0.09511867
  451    7    -2.89643    -0.54259     3.40496     -0.00078276    1.06930957   -
0.00073202   -0.11374352
  452    7    -4.50429    -0.54259     2.49837      0.00015085    2.14708963
0.00007026   -0.13629332
  453    5    -3.53552     0.54266     3.10112     -0.00134160    2.14708963   -
0.00062485   -0.12220240
  454    5    -5.05922     0.54266     2.05927      0.00076733    1.06930957
0.00071759   -0.14430118
  455    7    -5.05924    -0.54263    -2.05925      0.00075375    1.06930478
0.00070490   -0.14429371
  456    7    -3.53556    -0.54264    -3.10111     -0.00134034    2.14707981   -
0.00062426   -0.12220268
  457    5    -4.50431     0.54262    -2.49835      0.00015178    2.14707981
0.00007069   -0.13630561
  458    5    -2.89646     0.54260    -3.40496     -0.00078141    1.06930478   -
0.00073076   -0.11375025
  459    5    -0.38110     2.23591     3.39031     -0.00089696    0.28319697   -
0.00316726   -0.10218656
  460    8     0.38105     2.23591     3.39031     -0.00095318    0.28319697   -
0.00336579   -0.10218882
  461    9    -0.00003     1.86875     3.43263     -0.00129594    0.28319697   -
0.00457611   -0.09510354
  462    5    -0.38105     2.23594    -3.39032     -0.00097563    0.28319697   -
0.00344506   -0.10221664
  463    8     0.38109     2.23594    -3.39032     -0.00089055    0.28319697   -
0.00314465   -0.10220207
  464    9     0.00002     1.86878    -3.43264     -0.00133050    0.28319697   -
0.00469814   -0.09512234
  465    8     0.54264     2.89643    -3.40496     -0.00078241    1.06930158   -
0.00073170   -0.11373896
  466    8     0.54264     4.50429    -2.49837      0.00012206    2.14707344
0.00005685   -0.13629683
  467    5    -0.54261     3.53553    -3.10114     -0.00137470    2.14707344   -
0.00064027   -0.12225485
  468    5    -0.54261     5.05922    -2.05928      0.00083334    1.06930158
0.00077933   -0.14426709
  469    8     0.54261     5.05916     2.05936      0.00074961    1.06927619
0.00070105   -0.14428828
  470    8     0.54260     3.53548     3.10116     -0.00134242    2.14702141   -
0.00062525   -0.12219673
  471    5    -0.54264     4.50423     2.49842      0.00025862    2.14702141
0.00012046   -0.13630142
  472    5    -0.54265     2.89640     3.40496     -0.00082616    1.06927619   -
0.00077263   -0.11374338
  473    9    -1.10287     0.79727    -3.53978     -0.00497433    1.39408270   -
0.00356817   -0.08781259
  474    5    -1.33146     1.63912    -3.51869     -0.00258125    1.37765356   -
0.00187365   -0.10107663
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  475    9    -0.79730     1.10285     3.53977     -0.00523890    1.39400631   -
0.00375816   -0.08782425
  476    5    -1.63913     1.33147     3.51868     -0.00254533    1.37757806   -
0.00184769   -0.10102189
  477    6     0.38109    -2.23593     3.39031     -0.00088845    0.28319404   -
0.00313726   -0.10221923
  478    7    -0.38105    -2.23593     3.39032     -0.00096261    0.28319404   -
0.00339913   -0.10222783
  479    9     0.00002    -1.86878     3.43263     -0.00131041    0.28319404   -
0.00462726   -0.09514206
  480    6     0.38107    -2.23600    -3.39030     -0.00097507    0.28319404   -
0.00344311   -0.10217885
  481    7    -0.38108    -2.23600    -3.39030     -0.00090193    0.28319404   -
0.00318484   -0.10217438
  482    9    -0.00001    -1.86884    -3.43262     -0.00133157    0.28319404   -
0.00470196   -0.09508535
  483    7    -0.54264    -2.89648    -3.40493     -0.00083082    1.06929943   -
0.00077698   -0.11373557
  484    7    -0.54263    -4.50430    -2.49833      0.00025377    2.14706817
0.00011819   -0.13629615
  485    6     0.54263    -3.53557    -3.10110     -0.00135313    2.14706817   -
0.00063022   -0.12219972
  486    6     0.54263    -5.05922    -2.05924      0.00075773    1.06929943
0.00070863   -0.14430096
  487    7    -0.54261    -5.05918     2.05932      0.00082457    1.06929574
0.00077113   -0.14426307
  488    7    -0.54261    -3.53551     3.10115     -0.00136825    2.14706061   -
0.00063726   -0.12225626
  489    6     0.54265    -4.50425     2.49840      0.00012537    2.14706061
0.00005839   -0.13630895
  490    6     0.54265    -2.89642     3.40496     -0.00078044    1.06929574   -
0.00072986   -0.11375465
  491    6     2.23596    -0.38106    -3.39031     -0.00090939    0.28319682   -
0.00321116   -0.10218687
  492    8     2.23596     0.38108    -3.39031     -0.00098283    0.28319682   -
0.00347049   -0.10220309
  493    9     1.86880     0.00001    -3.43263     -0.00135954    0.28319682   -
0.00480070   -0.09510559
  494    6     2.23591    -0.38108     3.39032     -0.00096803    0.28319682   -
0.00341823   -0.10221796
  495    8     2.23591     0.38107     3.39032     -0.00090247    0.28319682   -
0.00318671   -0.10219717
  496    9     1.86875    -0.00001     3.43263     -0.00132465    0.28319682   -
0.00467750   -0.09511808
  497    8     2.89640     0.54263     3.40497     -0.00083220    1.06929624   -
0.00077827   -0.11374987
  498    8     4.50425     0.54264     2.49841      0.00022501    2.14706237
0.00010480   -0.13631056
  499    6     3.53550    -0.54262     3.10115     -0.00138577    2.14706237   -
0.00064542   -0.12225763
  500    6     5.05920    -0.54260     2.05932      0.00082697    1.06929624
0.00077338   -0.14427837
  501    8     5.05914     0.54266    -2.05938      0.00081812    1.06924858
0.00076513   -0.14427172
  502    8     3.53550     0.54265    -3.10115     -0.00138789    2.14696468   -
0.00064644   -0.12224430
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  503    6     4.50423    -0.54260    -2.49844     0.00022558    2.14696468
0.00010507   -0.13631699
  504    6     2.89644    -0.54261    -3.40496    -0.00084023    1.06924858   -
0.00078581   -0.11374089
  505    9     0.79729    -1.10286     3.53977    -0.00505395    1.39402123   -
0.00362545   -0.08785458
  506    6     1.63913    -1.33146     3.51868    -0.00253238    1.37759281   -
0.00183826   -0.10109067
  507    9     1.10287    -0.79731    -3.53977    -0.00526776    1.39409763   -
0.00377862   -0.08779489
  508    6     1.33147    -1.63916    -3.51867    -0.00256395    1.37766831   -
0.00186108   -0.10100076
  509    9    -0.79731    -1.10291    -3.53977    -0.00484001    1.39406430   -
0.00347187   -0.08777767
  510    7    -1.63916    -1.33150    -3.51867    -0.00257090    1.37763542   -
0.00186617   -0.10100583
  511    9    -1.10285    -0.79728     3.53977    -0.00508699    1.39405597   -
0.00364906   -0.08785614
  512    7    -1.33145    -1.63912     3.51869    -0.00251867    1.37762718   -
0.00182827   -0.10108440
  513    9     1.10282     0.79727     3.53978    -0.00497008    1.39403852   -
0.00356524   -0.08781715
  514    8     1.33143     1.63911     3.51869    -0.00248156    1.37760988   -
0.00180135   -0.10102015
  515    9     0.79731     1.10286    -3.53978    -0.00496366    1.39404685   -
0.00356061   -0.08782860
  516    8     1.63915     1.33146    -3.51868    -0.00259110    1.37761811   -
0.00188085   -0.10106049];
```

D.9.2 CATIONS

[BMPY] (Computation ID = 58)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.44
%   total number of segments         =    955
%   number of charge corr segments   =    386
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N            -0.05720166762315   -0.51851558683940    1.89905438762330   3.4582  -
0.0063     3.14    -0.00200    5.9148
% C            -1.68594314289758   -3.96854781562713   -0.97768186618969   3.7795  -
0.0087    20.81    -0.00042    6.2361
% C            -1.58321939196768   -2.89479305747911    1.70800439541529   3.7795  -
0.0375    25.11    -0.00149    6.2361
% C            -2.94644216739563   -2.25610895298214   -2.94621063262159   3.7795
0.0030    22.36     0.00014    6.2361
% C             2.50347603229416   -0.63741376634505    1.70287015504259   3.7795  -
0.0628    41.26    -0.00152    6.2361
% C            -1.20295936584941    1.75728615673788    2.20293591864558   3.7795  -
0.0583    36.58    -0.00159    6.2361
% C            -3.12502154510000   -3.51214239024066   -5.55018555421132   3.7795
0.0433    58.84     0.00074    6.2361
% C             2.84000845728422    3.91684514317335    2.11497388428353   3.7795  -
0.0175    19.45    -0.00090    6.2361
% C             3.96721792289638    1.52484940305748    1.80101240482218   3.7795  -
0.0323    44.94    -0.00072    6.2361
% C             0.19167780283042    3.96983559595118    2.31857386327189   3.7795  -
0.0327    45.05    -0.00073    6.2361
% C             4.39262452470312    6.28245461283950    2.19222054601752   3.7795  -
0.0230    56.87    -0.00041    6.2361
% H            -2.73209887239900   -5.76388566391377   -0.82576821730358   2.4566  -
0.0384    25.19    -0.00152    4.9133
% H             0.23525436759809   -4.49162421867468   -1.59614260357713   2.4566  -
0.0359    22.80    -0.00157    4.9133
% H            -3.47886425067859   -2.42896308413740    2.40653760972581   2.4566  -
0.0602    21.56    -0.00279    4.9133
% H            -0.74104459890306   -4.24990393974086    3.03522889349641   2.4566  -
0.0677    24.72    -0.00274    4.9133
% H            -1.88451291660560   -0.46921754174679   -3.11988372005682   2.4566  -
0.0273    20.26    -0.00135    4.9133
% H            -4.85950281766353   -1.74233986872966   -2.29245851718752   2.4566  -
0.0289    26.05    -0.00111    4.9133
```

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% H             3.30800938390311   -2.51818806026330    1.47456516092284   2.4566  -
0.0778    21.92    -0.00355    4.9133
% H            -3.25413289117765    1.72579273891891    2.35820630694477   2.4566  -
0.0776    22.34    -0.00347    4.9133
% H            -1.24357927268082   -4.01782208229591   -6.28190790940236   2.4566  -
0.0223    24.98    -0.00089    4.9133
% H            -4.01381323794136   -2.23837228025995   -6.92982418773503   2.4566  -
0.0246    24.29    -0.00101    4.9133
% H            -4.26226863684495   -5.25253927280422   -5.47486222171228   2.4566  -
0.0221    24.94    -0.00089    4.9133
% H             6.01567071125670    1.33260758136942    1.65355784629719   2.4566  -
0.0712    24.60    -0.00289    4.9133
% H            -0.81365960048619    5.75011448697859    2.58704402808724   2.4566  -
0.0698    24.26    -0.00288    4.9133
% H             4.87708387360900    6.87190653297877    0.25041950086941   2.4566  -
0.0507    24.99    -0.00203    4.9133
% H             6.18396142216122    5.98022834206299    3.20046507565893   2.4566  -
0.0475    24.10    -0.00197    4.9133
% H             3.36927987767774    7.84845698801208    3.08925545287296   2.4566  -
0.0457    23.46    -0.00195    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -445.409619
%   Total energy + OC corr.      =       -445.405044
%   Dielectric energy            =         -0.080386      -2.187      -50.44
%   Diel. energy + OC corr.      =         -0.075812      -2.063      -47.57
%
%   Surface area of cavity [au]
acosmo =           754.872;
%   Total Volume of cavity [au]
vcosmo =          1468.584;
%
%
% $screening_charge
%   cosmo           =   -1.03702
%   corrected total =   -1.00040
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1     0.19768    -0.67578     5.34426     -0.00005703    0.13889369   -
0.00041062    0.15839596
    2    1     0.29449    -1.48405     5.20105     -0.00027707    0.13889369   -
0.00199480    0.16294067
    3    1     0.03447    -1.00571     5.32153     -0.00026011    0.27778738   -
0.00093636    0.15993712
    4    2     0.17944    -7.24911    -0.77167      0.00062147    1.16128380
0.00053516    0.12314620
    5    2    -0.58314    -7.58298    -0.91558      0.00054691    0.82948843
0.00065933    0.11902048
    6    2    -1.70101    -7.26481    -2.82661     -0.00005272    0.16589769   -
0.00031778    0.11104366
```

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    7    2    -5.11354    -4.95409     0.27314     -0.00042698    0.49769306   -
0.00085792    0.13627542
    8    2    -0.48110    -7.04872    -2.80661      0.00056390    0.82948843
0.00067981    0.11098337
    9    2    -0.26143    -7.34284    -1.90991      0.00085040    1.16128380
0.00073229    0.11482040
   10    2    -0.05165    -7.12158     0.31526      0.00044429    1.16128380
0.00038259    0.13048057
   11    2     0.65652    -6.63086     0.32967     -0.00008205    0.82948843   -
0.00009891    0.13846662
   12    2    -0.86901    -7.35811     0.48099      0.00005124    0.82948843
0.00006177    0.13047395
   13    2    -1.11483    -7.44242    -2.35251      0.00044092    0.49769306
0.00088592    0.11142870
   14    2    -5.27662    -4.90608    -0.26189      0.00003859    0.16589769
0.00023263    0.13125283
   15    3    -3.70661    -5.81460     2.82619     -0.00064478    0.66359074   -
0.00097166    0.14205285
   16    3    -2.23672    -3.48666     5.38319     -0.00075052    1.32718149   -
0.00056550    0.15015213
   17    3    -3.16459    -3.53896     5.07976     -0.00027631    1.16128380   -
0.00023794    0.14824865
   18    3    -4.23001    -5.08565     3.28250     -0.00117395    1.16128380   -
0.00101090    0.14459213
   19    3    -4.56679    -5.11970     2.36563     -0.00074880    0.82948843   -
0.00090272    0.14517514
   20    3    -3.27363    -5.56638     3.77912     -0.00115540    1.32718149   -
0.00087057    0.14375261
   21    3    -3.06964    -4.55287     4.76181     -0.00051541    1.16128380   -
0.00044383    0.14534712
   22    3    -2.16982    -2.45112     5.41522     -0.00057610    0.99538612   -
0.00057877    0.15408254
   23    3    -2.79915    -6.29505     2.82341     -0.00103083    1.16128380   -
0.00088767    0.14488816
   24    3    -1.04417    -2.83544     5.44836     -0.00065234    0.66359074   -
0.00098305    0.15825404
   25    3    -0.58244    -2.41575     5.32093     -0.00022157    0.33179537   -
0.00066778    0.16214921
   26    3    -2.97939    -2.25977     5.16225     -0.00096836    0.82948843   -
0.00116742    0.15720113
   27    3    -3.77135    -4.70331     4.20315     -0.00050182    0.99538612   -
0.00050415    0.14470837
   28    3    -4.93629    -4.63862     1.68852     -0.00059973    0.33179537   -
0.00180753    0.14834576
   29    3    -1.38894    -2.18305     5.41476     -0.00064514    0.49769306   -
0.00129626    0.15821601
   30    4    -4.56257     0.69183    -4.67307      0.00084688    0.99538612
0.00085081    0.10284696
   31    4    -5.99166    -4.35964    -2.18058      0.00016868    0.33179537
0.00050837    0.11316014
   32    4    -3.68564     1.08551    -4.54975      0.00067110    0.82948843
0.00080905    0.10863808
   33    4     0.63787    -1.62575    -3.96578     -0.00008756    0.16589769   -
0.00052779    0.12708911
   34    4    -4.71054     0.99043    -3.74127      0.00113848    1.32718149
0.00085782    0.10858971
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   35    4    -4.66416     1.10554    -2.76480      0.00085452    0.82948843
0.00103018    0.11759901
   36    4    -5.43784     0.32579    -4.13405      0.00061844    0.82948843
0.00074556    0.10483489
   37    4    -6.00885    -4.17055    -1.83224      0.00001194    0.16589769
0.00007199    0.11727032
   38    4    -3.97327     1.37297    -3.19019      0.00047423    0.49769306
0.00095286    0.11699424
   39    4     0.48397    -1.30989    -4.21945     -0.00005842    0.16589769   -
0.00035212    0.12486899
   40    5     2.09101    -0.18353     5.43221     -0.00055625    0.66359074   -
0.00083824    0.14818881
   41    5     4.88203    -1.91289     4.34860     -0.00017655    1.16128380   -
0.00015203    0.14866233
   42    5     3.59084    -1.33497    -1.84896     -0.00053857    0.66359074   -
0.00081160    0.14776762
   43    5     4.16408    -2.18264    -1.32023     -0.00131649    0.82948843   -
0.00158712    0.15665930
   44    5     4.95185    -2.60649     3.80345     -0.00093078    0.66359074   -
0.00140264    0.15744965
   45    5     5.79378    -2.05253     0.49634     -0.00153076    0.66359074   -
0.00230678    0.16993988
   46    5     5.51940    -2.29003     3.27046     -0.00108420    0.66359074   -
0.00163383    0.16027126
   47    5     4.12208    -2.43480     4.60696     -0.00089537    1.16128380   -
0.00077101    0.15058168
   48    5     3.08602    -2.89244     4.67939     -0.00115752    0.99538612   -
0.00116288    0.15733971
   49    5     4.41931    -1.33839    -1.47874     -0.00066269    0.99538612   -
0.00066576    0.14928403
   50    5     5.14901    -1.68571    -0.78443     -0.00005318    0.66359074   -
0.00008013    0.15727916
   51    5     4.02475    -1.40858     5.07558     -0.00024524    1.16128380   -
0.00021118    0.14310330
   52    5     2.95858    -0.73035     5.45365      0.00004026    1.16128380
0.00003467    0.14334157
   53    5     1.94232    -0.94439     5.42778     -0.00051699    0.66359074   -
0.00077908    0.15077230
   54    5     2.12229    -1.89805     5.24542     -0.00168781    1.16128380   -
0.00145340    0.15463715
   55    5     3.44241    -0.57952    -1.95766     -0.00009126    0.99538612   -
0.00009169    0.14388865
   56    5     3.65930    -3.25255     4.17458     -0.00162907    0.99538612   -
0.00163662    0.16176781
   57    5     5.81040    -2.26628     2.53678     -0.00071123    0.33179537   -
0.00214359    0.16704920
   58    5     5.01739    -2.24348    -0.61773     -0.00119304    0.66359074   -
0.00179786    0.16322191
   59    5     2.77485    -0.19043    -2.04025     -0.00057223    0.49769306   -
0.00114977    0.14405914
   60    5     3.02848    -1.88152     5.23285     -0.00102353    1.32718149   -
0.00077121    0.14852713
   61    6    -3.34849     3.70050    -0.22706     -0.00033856    0.66359074   -
0.00051020    0.14978374
   62    6    -2.67310     1.57133     5.67976     -0.00100558    1.32718149   -
0.00075768    0.14982987
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   63    6    -3.42714     2.12443     5.23648     -0.00156865    1.16128380   -
0.00135079    0.15579623
   64    6    -3.91687     3.34369     0.10479     -0.00094487    0.66359074   -
0.00142388    0.15653222
   65    6    -3.86412     4.12147     3.47302     -0.00154849    0.66359074   -
0.00233350    0.16903873
   66    6    -3.87445     3.95474     0.68025     -0.00131906    0.66359074   -
0.00198777    0.15955477
   67    6    -3.63407     2.96938    -0.42476     -0.00103017    0.66359074   -
0.00155242    0.15141395
   68    6    -2.62499     0.49889     5.47072     -0.00106161    0.99538612   -
0.00106653    0.15720809
   69    6    -2.72906     2.93986     5.45206     -0.00079236    1.16128380   -
0.00068232    0.14746227
   70    6    -3.31349     3.59603     4.74241     -0.00002011    0.66359074   -
0.00003030    0.15601191
   71    6    -2.72060     3.56114    -0.75124     -0.00005868    0.49769306   -
0.00011791    0.14440553
   72    6    -0.64598     0.51826     5.72981     -0.00073815    0.82948843   -
0.00088989    0.15100058
   73    6    -1.63963     0.81860     5.83782     -0.00155935    1.65897686   -
0.00093995    0.14959083
   74    6    -1.72541     2.24112     5.91470     -0.00000232    1.49307918   -
0.00000156    0.14219975
   75    6    -3.51484     0.85125     5.05223     -0.00194700    0.99538612   -
0.00195603    0.16418891
   76    6    -3.99539     4.18291     1.42647     -0.00046484    0.33179537   -
0.00140097    0.16609704
   77    6    -3.71193     3.18947     4.63976     -0.00089712    0.82948843   -
0.00108153    0.16053467
   78    6    -0.43076     1.44621     5.88956     -0.00073756    1.49307918   -
0.00049399    0.14417050
   79    7    -2.20388    -7.14723    -6.02108      0.00113969    0.82948843
0.00137397    0.08266989
   80    7    -3.11345    -4.68870    -9.14180      0.00125722    1.32718149
0.00094728    0.06873914
   81    7    -1.56305    -1.21402    -8.11204      0.00190128    1.49307918
0.00127340    0.08288905
   82    7    -6.87473    -3.74109    -5.13599      0.00160034    1.49307918
0.00107184    0.08575826
   83    7    -6.78926    -4.22014    -6.14710      0.00080307    0.66359074
0.00121019    0.07938759
   84    7    -6.77933    -2.56081    -5.39103      0.00091702    0.82948843
0.00110553    0.08638162
   85    7    -6.77484    -2.69266    -6.09014      0.00086539    0.82948843
0.00104328    0.08243798
   86    7     0.26281    -1.86014    -5.82909      0.00028153    0.33179537
0.00084852    0.10716708
   87    7    -0.87460    -2.03156    -8.20117      0.00128113    0.99538612
0.00128707    0.08269267
   88    7    -1.99868    -4.75271    -8.93787      0.00126529    1.49307918
0.00084744    0.07319580
   89    7    -1.52324    -6.84105    -6.34817      0.00111038    0.82948843
0.00133863    0.08267140
   90    7    -6.20674    -4.50452    -7.50015      0.00179410    1.32718149
0.00135181    0.07284111
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   91    7    -6.24987    -3.79814    -7.65677      0.00111953    0.82948843
0.00134966    0.07368199
   92    7    -1.88669    -7.05675    -5.11842      0.00140652    0.99538612
0.00141304    0.08906522
   93    7    -2.39762    -6.81302    -7.24110      0.00237765    1.82487455
0.00130291    0.07605484
   94    7    -2.79554    -5.83813    -8.51081      0.00152637    1.49307918
0.00102230    0.07032021
   95    7    -2.70727    -3.50661    -9.30646      0.00167759    1.49307918
0.00112358    0.07151619
   96    7    -1.85592    -2.28122    -8.89060      0.00193073    1.32718149
0.00145476    0.07636893
   97    7    -0.83172    -1.02139    -7.22982      0.00185366    1.65897686
0.00111735    0.08968072
   98    7    -0.31710    -1.10341    -6.32341      0.00065421    0.66359074
0.00098586    0.09919220
   99    7    -5.09879    -5.35097    -8.19727      0.00134747    1.32718149
0.00101529    0.07104810
  100    7    -4.09341    -5.16867    -8.80629      0.00159418    1.65897686
0.00096094    0.06832008
  101    7    -3.94636    -3.96001    -9.21201      0.00082967    0.99538612
0.00083352    0.07087153
  102    7    -2.01292    -0.27321    -7.14920      0.00058489    0.66359074
0.00088140    0.09186578
  103    7    -2.54056     0.09041    -6.53220      0.00024942    0.33179537
0.00075174    0.09702322
  104    7    -6.62724    -4.23967    -4.32976      0.00043715    0.66359074
0.00065877    0.09353896
  105    7    -6.76510    -3.50644    -6.56707      0.00178524    1.32718149
0.00134514    0.07722623
  106    7    -6.41605    -1.65859    -5.68354      0.00043116    0.49769306
0.00086631    0.09034943
  107    7    -0.10204    -1.55069    -6.68973      0.00036540    0.49769306
0.00073419    0.09746786
  108    7    -1.75385    -3.33151    -9.06748      0.00148271    1.16128380
0.00127679    0.07411031
  109    7    -2.03117    -6.15790    -8.01748      0.00103802    0.99538612
0.00104283    0.07465532
  110    7    -1.09374    -6.69291    -5.34826      0.00082272    0.66359074
0.00123980    0.09108572
  111    7    -5.16774    -4.33704    -8.62118      0.00172593    1.49307918
0.00115596    0.07026092
  112    7    -3.69837    -6.19269    -8.15211      0.00106602    1.16128380
0.00091796    0.07168663
  113    7    -1.52369    -0.29647    -6.72470      0.00074148    0.66359074
0.00111738    0.09434102
  114    8     2.68586     4.51346     5.84386     -0.00032713    0.49769306   -
0.00065729    0.13299504
  115    8     3.94071     3.60291     5.71695     -0.00013311    0.82948843   -
0.00016048    0.13337864
  116    8     3.22072     4.01912     5.87382      0.00015660    0.66359074
0.00023599    0.13227261
  117    8     2.46404     3.75990     5.87242      0.00080418    0.49769306
0.00161581    0.13261977
  118    8     2.34270     3.72444    -1.62667     -0.00062871    1.32718149   -
0.00047372    0.13816411
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  119    8     3.19479     4.13795    -1.64127     -0.00003428    0.82948843   -
0.00004133    0.13853272
  120    8     2.12946     4.83650    -1.48135     -0.00017982    0.82948843   -
0.00021679    0.13768733
  121    8     2.95421     3.02747     5.78653      0.00027371    0.99538612
0.00027498    0.13338497
  122    9     3.20895     1.19525     5.48891      0.00017707    0.33179537
0.00053369    0.13673470
  123    9     5.74314     2.20963     5.06617     -0.00017384    0.49769306   -
0.00034930    0.13608723
  124    9     6.07412    -0.44345     4.24457     -0.00026101    0.99538612   -
0.00026222    0.14314918
  125    9     5.38950     1.76569    -1.69233     -0.00014545    1.32718149   -
0.00010959    0.13526659
  126    9     6.30108     1.69049    -1.16714     -0.00077922    1.16128380   -
0.00067100    0.14201768
  127    9     6.30594    -0.71460    -0.14825     -0.00012809    0.33179537   -
0.00038606    0.15845127
  128    9     6.54204    -0.70166     3.44334     -0.00054004    0.99538612   -
0.00054255    0.15286673
  129    9     6.63255     1.92994     4.44980     -0.00072750    0.82948843   -
0.00087704    0.14239654
  130    9     6.02612     1.50504     4.97035     -0.00008787    0.82948843   -
0.00010593    0.13544408
  131    9     5.95848     0.29857     4.77007     -0.00006129    0.82948843   -
0.00007389    0.13671961
  132    9     6.10558    -0.31138    -0.71693     -0.00061426    0.66359074   -
0.00092566    0.15080560
  133    9     5.48964     0.51466    -1.50748      0.00021202    1.49307918
0.00014200    0.13925998
  134    9     5.81167     2.72824    -1.27048     -0.00047932    0.82948843   -
0.00057785    0.13926013
  135    9     5.03161     1.85971     5.41198      0.00004909    1.16128380
0.00004227    0.13250854
  136    9     3.95434     1.57388     5.58011      0.00045142    0.82948843
0.00054421    0.13245876
  137    9     4.16313     0.80191     5.50549      0.00050211    0.82948843
0.00060532    0.13268557
  138    9     5.07948     0.04973     5.09815      0.00057079    0.99538612
0.00057343    0.13511156
  139    9     4.32520     1.20194    -1.94758      0.00053334    1.82487455
0.00029226    0.13452670
  140    9     4.51869     2.58321    -1.78508     -0.00019619    1.49307918   -
0.00013140    0.13496816
  141    9     6.21293     0.46944    -1.04982     -0.00053494    0.82948843   -
0.00064490    0.14503873
  142    9     6.57062     0.79217     4.44102     -0.00073933    1.16128380   -
0.00063665    0.14119637
  143    9     6.53155     2.68713    -0.72041     -0.00048535    0.49769306   -
0.00097520    0.14575239
  144    9     3.32078     2.03424    -1.88775      0.00019050    1.32718149
0.00014353    0.13580461
  145    9     5.23524     0.90182     5.30645      0.00012099    0.99538612
0.00012156    0.13221248
  146   10     0.18021     6.32081    -0.64067      0.00006436    0.82948843
0.00007759    0.13630673
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  147   10    -2.39892     5.30356    -0.08854     -0.00015686    0.99538612   -
0.00015759    0.14293034
  148   10    -0.24690     5.08065     5.90436     -0.00008083    1.32718149   -
0.00006090    0.13269534
  149   10    -0.40155     6.04118     5.42369     -0.00092162    0.99538612   -
0.00092589    0.14029728
  150   10    -2.84764     5.04970     4.28848     -0.00008799    0.33179537   -
0.00026519    0.15711442
  151   10    -2.84339     5.56220     0.72580     -0.00060525    0.99538612   -
0.00060806    0.15239374
  152   10    -0.31316     6.97720     0.08582     -0.00086498    0.82948843   -
0.00104278    0.14297538
  153   10    -0.60221     6.17533    -0.64620     -0.00015727    0.99538612   -
0.00015800    0.13539549
  154   10    -1.66071     5.53775    -0.57877     -0.00008518    0.82948843   -
0.00010269    0.13679741
  155   10    -2.27956     5.05482     4.96431     -0.00097872    0.99538612   -
0.00098326    0.14787102
  156   10    -1.47020     4.60517     5.65303      0.00024273    1.32718149
0.00018289    0.13747924
  157   10     0.47358     5.88559     5.56427     -0.00051126    0.82948843   -
0.00061635    0.13682932
  158   10     0.22804     5.32034    -1.21118      0.00005212    1.32718149
0.00003927    0.13340561
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  947   26     8.09829     4.29229     2.69552     -0.00351015    2.01313758   -
0.00174362    0.14279629
  948   23     7.86718     2.62062     2.95035     -0.00489833    2.01313758   -
0.00243318    0.15327138
  949   23     8.09538     3.01183     1.75011     -0.00166825    1.00674570   -
0.00165708    0.15044796
  950   27     1.12511     8.90290     2.09739     -0.00079948    0.77168762   -
0.00103602    0.13916797
  951   27     0.98326     8.93885     3.12862     -0.00281338    1.54259243   -
0.00182380    0.14246630
  952   27     1.10535     8.41833     4.28655     -0.00263361    1.54259243   -
0.00170726    0.14342313
  953   24    -0.22517     8.29426     2.33317     -0.00359492    1.54259243   -
0.00233044    0.15182630
  954   24    -0.28647     8.11460     3.59437     -0.00377546    1.54259243   -
0.00244748    0.15199003
  955   24    -0.09748     7.53562     4.43930     -0.00136957    0.77168762   -
0.00177477    0.14937623];
```

[EMIM] (Computation ID = 59)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.44
%   total number of segments         =    711
%   number of charge corr segments   =    301
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N            -1.00130988104902   -0.49630790346316   -0.60427467685015   3.4582  -
0.0038     3.67    -0.00104    5.9148
% N             2.32632892512309    1.96496124119820   -0.54673656224772   3.4582  -
0.0082     6.25    -0.00131    5.9148
% C            -2.60000519848539   -2.80142500432226   -0.51820741607158   3.7795  -
0.0400    28.77    -0.00139    6.2361
% C             1.54162580011089   -0.45583885913749   -0.58986917743630   3.7795  -
0.0770    47.38    -0.00162    6.2361
% C            -1.86345149956333    1.97642508710122   -0.56494553233061   3.7795  -
0.0343    48.54    -0.00071    6.2361
% C             0.21623413228059    3.51658604143988   -0.53610996517356   3.7795  -
0.0419    52.84    -0.00079    6.2361
% C            -3.33650181067095   -3.53339764428992    2.17379464472465   3.7795  -
0.0058    60.39    -0.00010    6.2361
% C             4.97485261888001    2.81328457379474   -0.62407346974253   3.7795  -
0.0810    63.36    -0.00128    6.2361
% H            -1.52758622726389   -4.30802082464249   -1.45684530686262   2.4566  -
0.0632    23.84    -0.00265    4.9133
% H            -4.26441449280945   -2.40391248544037   -1.68928960999889   2.4566  -
0.0618    24.22    -0.00255    4.9133
% H             2.76311953757325   -2.10103319901438   -0.61548051655559   2.4566  -
0.1097    27.68    -0.00396    4.9133
% H            -3.86181792090129    2.43365376411514   -0.55644765126501   2.4566  -
0.0858    26.02    -0.00330    4.9133
% H             0.36842537248582    5.56132987945249   -0.51925475709211   2.4566  -
0.0832    24.60    -0.00338    4.9133
% H            -4.52509615706981   -5.23580965413076    2.10562527109372   2.4566  -
0.0405    24.28    -0.00167    4.9133
% H            -4.42238702506121   -2.02787299443665    3.10688200170575   2.4566  -
0.0372    23.50    -0.00158    4.9133
% H            -1.66434360933368   -3.95865923229329    3.33155653903184   2.4566  -
0.0376    23.99    -0.00157    4.9133
% H             5.45787217411291    3.42122404366278   -2.54763833842074   2.4566  -
0.0623    25.14    -0.00248    4.9133
% H             6.20206898940025    1.24787856406187   -0.05027914942219   2.4566  -
0.0637    23.25    -0.00274    4.9133
```

```
% H             5.21638627224118    4.38693460634448    0.70159367291364   2.4566  -
0.0631    24.25    -0.00260    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -344.705810
%   Total energy + OC corr.      =       -344.701551
%   Dielectric energy            =         -0.084558      -2.301      -53.06
%   Diel. energy + OC corr.      =         -0.080299      -2.185      -50.39
%
%   Surface area of cavity [au]
acosmo =           581.961;
%   Total Volume of cavity [au]
vcosmo =          1059.419;
%
%
% $screening_charge
%   cosmo           =   -1.02946
%   corrected total =   -1.00008
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1    -1.24982    -0.68711    -4.04825      0.00004985    0.69446845
0.00007178    0.15268459
    2    1    -1.01776    -0.21881    -4.05129     -0.00003148    0.13889369   -
0.00022665    0.15130409
    3    2     2.56915     2.09756     2.90040      0.00005941    0.55557476
0.00010694    0.15444141
    4    2     2.18104     2.07554    -4.00010     -0.00014485    0.13889369   -
0.00104292    0.15837004
    5    2     2.54550     1.92232    -3.99770     -0.00009270    0.13889369   -
0.00066745    0.16001201
    6    2     2.10739     2.00761     2.90428     -0.00006956    0.13889369   -
0.00050085    0.15334142
    7    3    -4.33463    -5.94007    -1.71166     -0.00086280    0.99538612   -
0.00086680    0.13837293
    8    3    -3.11731    -3.33157    -4.22436     -0.00057868    1.32718149   -
0.00043602    0.14521724
    9    3    -2.61013    -4.21270    -4.02426     -0.00041430    0.99538612   -
0.00041622    0.14613488
   10    3    -3.72790    -5.89947    -2.36597     -0.00085702    0.99538612   -
0.00086100    0.14114571
   11    3    -3.52473    -6.36197    -1.38523     -0.00063554    0.66359074   -
0.00095773    0.14203498
   12    3    -4.57081    -5.13522    -2.74388     -0.00074354    1.16128380   -
0.00064027    0.13940802
   13    3    -3.77687    -4.42882    -3.71989     -0.00039881    1.32718149   -
0.00030050    0.14137188
   14    3    -2.24946    -2.90694    -4.27987     -0.00060751    1.16128380   -
0.00052314    0.14874955
   15    3    -1.38116    -2.55091    -4.08693     -0.00069647    0.66359074   -
0.00104955    0.15582567
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   16    3    -5.16565    -5.24881    -1.82667     -0.00101480    1.16128380   -
0.00087386    0.13912478
   17    3    -3.03284    -1.91152    -4.16580     -0.00070674    0.66359074   -
0.00106502    0.15286090
   18    3    -1.34731    -3.28560    -4.05098     -0.00078576    0.82948843   -
0.00094728    0.15633633
   19    3    -3.66916    -5.24728    -3.19383     -0.00049269    0.99538612   -
0.00049497    0.14069422
   20    3    -2.98721    -6.54701    -0.84217     -0.00038368    0.33179537   -
0.00115639    0.14485978
   21    3    -5.74561    -4.71954    -1.36107     -0.00034631    0.49769306   -
0.00069582    0.14169198
   22    3    -2.38686    -1.85896    -4.17204     -0.00040585    0.66359074   -
0.00061159    0.15259576
   23    4     1.10497     0.40536     3.06415     -0.00123625    0.82948843   -
0.00149038    0.15510853
   24    4     3.68988    -1.08181     2.45601     -0.00135614    0.99538612   -
0.00136243    0.16846115
   25    4     2.61352    -1.64915    -4.01206     -0.00124920    1.32718149   -
0.00094124    0.16172426
   26    4     3.22157    -2.23108    -3.47269     -0.00174010    0.99538612   -
0.00174816    0.17156208
   27    4     3.92552    -1.90407     1.96040     -0.00163948    0.82948843   -
0.00197649    0.17777230
   28    4     3.10248    -1.60886     2.65335     -0.00097805    0.99538612   -
0.00098258    0.16506345
   29    4     2.73031    -2.21435     2.53726     -0.00068334    0.49769306   -
0.00137301    0.16724510
   30    4     1.87944    -2.50891    -3.74505     -0.00121793    1.16128380   -
0.00104878    0.16620699
   31    4     3.69720    -1.26416    -3.58727     -0.00071492    0.99538612   -
0.00071824    0.16833203
   32    4     2.78394    -0.22557     2.97212     -0.00117830    1.49307918   -
0.00078918    0.15906500
   33    4     1.77240     0.00426     3.15436     -0.00088524    0.99538612   -
0.00088934    0.15514686
   34    4     0.69936    -0.42861    -4.27419     -0.00087525    1.16128380   -
0.00075369    0.15475285
   35    4     1.59351    -1.12862    -4.30861     -0.00113570    1.49307918   -
0.00076064    0.15652913
   36    4     2.66641    -0.39179    -4.19751     -0.00184232    1.82487455   -
0.00100956    0.15907473
   37    4     2.33155    -3.04140    -3.23094     -0.00191100    0.99538612   -
0.00191986    0.17634101
   38    4     3.00058    -2.66216     2.10973     -0.00114619    0.49769306   -
0.00230300    0.17548700
   39    4     4.17025    -1.72284    -2.99181     -0.00120834    0.66359074   -
0.00182091    0.17902506
   40    4     1.46433     0.32778    -4.28639     -0.00152927    1.49307918   -
0.00102424    0.15569999
   41    4     2.19020    -1.14439     3.06929     -0.00122540    1.16128380   -
0.00105521    0.15846339
   42    4     0.96206    -1.82562    -4.06437     -0.00098768    0.99538612   -
0.00099226    0.16015552
   43    5    -3.21699     4.40648     1.99374      0.00021899    1.16128380
0.00018857    0.13820802
```

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   44    5    -3.68592     4.95170    -2.01773     -0.00110311    0.99538612   -
0.00110822    0.14933990
   45    5    -3.42276     2.34013    -3.98849      0.00003722    1.49307918
0.00002493    0.13592027
   46    5    -4.34870     2.44047    -3.37431     -0.00090325    1.16128380   -
0.00077781    0.14663071
   47    5    -3.75256     5.21474    -1.04326     -0.00086662    0.66359074   -
0.00130596    0.15581519
   48    5    -4.01774     4.00408     1.78702     -0.00099003    0.99538612   -
0.00099461    0.14557572
   49    5    -3.57843     2.51403     2.75980     -0.00023870    0.66359074   -
0.00035970    0.13790117
   50    5    -3.48240     3.36934     2.55321      0.00006262    0.99538612
0.00006291    0.13571032
   51    5    -3.65393     4.86219     1.09358     -0.00063334    0.82948843   -
0.00076353    0.14853598
   52    5    -3.57317     5.32084    -0.14548     -0.00064073    0.33179537   -
0.00193111    0.15559783
   53    5    -3.40336     4.55489    -2.85939     -0.00034067    1.16128380   -
0.00029336    0.14017709
   54    5    -3.75156     3.38461    -3.52068     -0.00005565    1.16128380   -
0.00004792    0.13730777
   55    5    -4.00476     1.36867    -3.61941     -0.00013357    0.82948843   -
0.00016103    0.14785441
   56    5    -1.31788     1.65728     3.16127      0.00022763    0.66359074
0.00034303    0.13710608
   57    5    -1.68689     2.45662     3.17970      0.00079265    0.82948843
0.00095559    0.13094611
   58    5    -2.53672     3.46301     2.84399      0.00109158    1.16128380
0.00093998    0.12956079
   59    5    -2.22925     2.67797    -4.26067      0.00159201    1.65897686
0.00095964    0.12944414
   60    5    -2.90418     1.40516    -4.15311     -0.00024546    1.32718149   -
0.00018495    0.13925913
   61    5    -2.26397     0.93357    -4.17554     -0.00015291    0.82948843   -
0.00018434    0.14202026
   62    5    -4.10298     3.95918    -2.87523     -0.00071163    0.82948843   -
0.00085791    0.14549156
   63    5    -3.82431     5.07547     0.34891     -0.00111143    0.49769306   -
0.00223316    0.15483760
   64    5    -4.25062     2.95586     2.19661     -0.00059464    0.66359074   -
0.00089609    0.14600682
   65    5    -4.73646     1.55163    -2.98355     -0.00074502    0.33179537   -
0.00224541    0.15838374
   66    5    -1.40772     1.60698    -4.29861      0.00057851    1.49307918
0.00038746    0.13728695
   67    5    -2.54546     2.50136     3.11519      0.00058699    1.16128380
0.00050546    0.13164806
   68    5    -2.84758     3.72456    -3.76804      0.00105173    1.16128380
0.00090566    0.13034116
   69    6     1.46990     4.92088    -3.81340     -0.00036123    0.49769306   -
0.00072582    0.14682297
   70    6    -1.73142     5.55960    -3.04947      0.00019188    1.16128380
0.00016523    0.13782975
   71    6    -2.07536     6.11561     0.97316     -0.00125752    0.99538612   -
0.00126335    0.14969327
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   72    6     0.36151     5.06873     2.90686      0.00002404    1.49307918
0.00001610    0.13703953
   73    6     0.53265     5.99111     2.30307     -0.00088894    1.16128380   -
0.00076548    0.14771428
   74    6    -2.31648     6.26960     0.00293     -0.00060745    0.66359074   -
0.00091540    0.15594945
   75    6    -1.10887     6.20344    -2.84029     -0.00094210    0.99538612   -
0.00094647    0.14506685
   76    6     1.53181     5.92273    -3.13690     -0.00150936    0.99538612   -
0.00151635    0.15519933
   77    6     0.84204     5.40701    -3.74843     -0.00031153    0.99538612   -
0.00031297    0.14267816
   78    6    -0.57805     5.48946    -3.66040      0.00025604    1.16128380
0.00022048    0.13510904
   79    6    -2.02934     6.09955    -2.13921     -0.00049639    0.82948843   -
0.00059843    0.14822914
   80    6    -2.47942     6.14125    -0.89509     -0.00073831    0.33179537   -
0.00222521    0.15562050
   81    6    -1.77136     5.71764     1.80677     -0.00025075    1.16128380   -
0.00021592    0.14071811
   82    6    -0.54411     5.69682     2.45601     -0.00003059    1.16128380   -
0.00002634    0.13812678
   83    6     1.45775     5.34344     2.53075     -0.00012056    0.82948843   -
0.00014535    0.14946626
   84    6     1.06503     4.17393    -4.15989     -0.00010854    1.32718149   -
0.00008178    0.14134948
   85    6     0.62312     3.02839    -4.26175      0.00019070    1.49307918
0.00012772    0.14049247
   86    6    -0.30032     3.67782    -4.27662      0.00122988    1.16128380
0.00105907    0.13089892
   87    6    -1.03868     4.64277    -3.91859      0.00106969    1.16128380
0.00092112    0.12928090
   88    6    -0.31051     4.02430     3.17186      0.00159363    1.65897686
0.00096061    0.13017894
   89    6     1.10359     4.29557     3.05417     -0.00025470    1.32718149   -
0.00019191    0.14073461
   90    6     1.36569     3.54458     3.06420     -0.00017032    0.82948843   -
0.00020533    0.14354336
   91    6    -0.99576     6.21040     1.82159     -0.00082669    0.82948843   -
0.00099662    0.14613356
   92    6    -2.17571     6.31541    -1.39019     -0.00116813    0.49769306   -
0.00234710    0.15478432
   93    6     0.16935     6.01535    -3.37131     -0.00082691    1.16128380   -
0.00071206    0.14456571
   94    6     1.49247     6.10486     1.90448     -0.00058231    0.33179537   -
0.00175503    0.15982468
   95    6     0.47101     2.92324     3.18777      0.00051157    1.49307918
0.00034263    0.13804669
   96    6     0.04325     4.61063    -4.14962      0.00036376    1.16128380
0.00031324    0.13309466
   97    6    -1.13303     4.92998     2.69902      0.00103874    1.16128380
0.00089448    0.13101529
   98    7    -2.08338    -6.76477     3.68116      0.00072680    0.82948843
0.00087621    0.11357943
   99    7    -4.92495    -4.45933     5.47589      0.00052826    1.32718149
0.00039803    0.10238149
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  100    7    -7.06794    -3.20089     2.67393      0.00100579    1.32718149
0.00075784    0.11383366
  101    7    -1.32835    -1.45674     4.61085      0.00026655    0.66359074
0.00040167    0.13034779
  102    7    -7.04401    -4.14240     2.58336      0.00054028    0.99538612
0.00054278    0.11253689
  103    7    -5.36470    -5.28801     4.83689      0.00027821    1.49307918
0.00018633    0.10471765
  104    7    -2.70862    -7.10726     3.23090      0.00078972    1.32718149
0.00059504    0.11317448
  105    7    -2.95503    -6.99602     0.70791     -0.00012771    0.66359074   -
0.00019246    0.13214465
  106    7    -2.32901    -2.10218     5.52357      0.00102329    1.32718149
0.00077102    0.11738232
  107    7    -2.80108    -1.57630     5.36245      0.00053992    0.82948843
0.00065090    0.11894206
  108    7    -1.95398    -6.95828     1.37196      0.00031872    0.99538612
0.00032020    0.12748399
  109    7    -1.60413    -6.87557     2.50992      0.00086711    1.32718149
0.00065335    0.12091033
  110    7    -2.92901    -6.42094     4.57803      0.00123678    1.82487455
0.00067773    0.10772149
  111    7    -4.05578    -5.48119     5.33181      0.00071923    1.49307918
0.00048171    0.10301278
  112    7    -5.91290    -3.91525     4.91254      0.00079870    1.49307918
0.00053494    0.10480476
  113    7    -6.76491    -3.66261     3.75924      0.00099023    1.16128380
0.00085270    0.10820390
  114    7    -7.04794    -3.62784     1.46630      0.00064950    1.16128380
0.00055929    0.11906520
  115    7    -6.80071    -3.62030     0.66518      0.00035711    0.49769306
0.00071752    0.12696753
  116    7    -0.27069    -5.71540     1.82191     -0.00024787    0.49769306   -
0.00049805    0.14628091
  117    7    -2.88775    -3.50059     5.92639      0.00053500    1.32718149
0.00040311    0.11032659
  118    7    -3.82658    -4.20740     5.86025      0.00066504    1.65897686
0.00040088    0.10433092
  119    7    -4.83611    -3.38283     5.63976      0.00033591    1.16128380
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0.00163515    0.12638634
  592   14    -3.69630    -7.25252     3.12275     -0.00090285    0.52699492   -
0.00171320    0.11915244
  593   14    -4.52401    -6.71005     4.00698     -0.00087227    0.52699492   -
0.00165518    0.11539092
  594   14    -5.60987    -5.95680     4.12848     -0.00098322    0.52699492   -
0.00186571    0.11439742
  595   14    -6.52673    -5.28908     3.43947     -0.00088897    0.52699492   -
0.00168686    0.11578656
  596   14    -6.91393    -4.96953     2.21097     -0.00090065    0.52699492   -
0.00170903    0.12068058
  597   14    -6.61916    -5.12386     0.92625     -0.00098347    0.52699492   -
0.00186619    0.12922785
  598    7    -3.21205    -7.10467     1.08255     -0.00074935    0.52047648   -
0.00143973    0.13125583
  599    7    -3.09912    -7.24255     2.55614     -0.00052804    0.52047648   -
0.00101453    0.12032563
  600    7    -3.73028    -6.85340     3.84200     -0.00044334    0.52047648   -
0.00085179    0.11364856
  601    7    -4.85727    -6.09030     4.43432     -0.00067352    0.52047648   -
0.00129404    0.11148958
  602    7    -6.03675    -5.25343     4.10009     -0.00059203    0.52047648   -
0.00113747    0.11151264
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0.00087493    0.11479347
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  606   15    -6.39091    -1.14145     1.93495     -0.00054883    0.24487021   -
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  607   15    -6.78184    -1.88605     2.68144     -0.00094387    0.54481555   -
0.00173246    0.12975771
  608   15    -6.64331    -2.52517     3.87389     -0.00087294    0.54481555   -
0.00160227    0.12070424
  609   15    -5.83151    -2.61365     4.96143     -0.00092579    0.54481555   -
0.00169927    0.11826821
  610   15    -4.68329    -2.11480     5.49277     -0.00098551    0.54481555   -
0.00180889    0.12035116
  611   15    -3.67512    -1.23560     5.24745     -0.00084542    0.54481555   -
0.00155175    0.12635763
  612   15    -3.20338    -0.47407     4.56771     -0.00042911    0.24487021   -
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  613    7    -6.57802    -1.70473     1.88841     -0.00076826    0.53213920   -
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  618    7    -2.99249    -0.95402     4.84990     -0.00057111    0.53213920   -
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  619   16    -0.66981    -2.11954     4.62487     -0.00039100    0.23502878   -
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  621   16    -1.85281    -3.77570     5.72519     -0.00081556    0.51846975   -
0.00157300    0.12280621
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  623   16    -1.64769    -5.99737     4.61288     -0.00081940    0.51846975   -
0.00158042    0.12202743
  624   16    -0.96050    -6.25322     3.52636     -0.00081683    0.51846975   -
0.00157546    0.12958452
  625   16    -0.19012    -5.72036     2.60941     -0.00104866    0.51846975   -
0.00202261    0.14459532
  626    7    -1.20237    -2.01150     4.83900     -0.00051096    0.51489634   -
0.00099236    0.13251253
  627    7    -1.98539    -2.97838     5.61479     -0.00048632    0.51489634   -
0.00094451    0.12165340
  628    7    -2.39498    -4.38423     5.68999     -0.00060332    0.51489634   -
0.00117173    0.11672560
  629    7    -2.27434    -5.69087     5.03579     -0.00046217    0.51489634   -
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  630    7    -1.66966    -6.39810     3.90265     -0.00045989    0.51489634   -
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0.00109542    0.13332006
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  635   18     6.09415    -0.80459    -1.59299     -0.00111244    0.31332013   -
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  636   11     4.94687    -1.93068    -2.02263     -0.00115487    0.35312529   -
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  637    8     5.84964    -0.77818    -2.18243     -0.00040787    0.50589743   -
0.00080624    0.17317367
  638    8     3.93451     6.50508    -0.42261     -0.00083106    0.29969230   -
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  640   19     4.03377     6.53785    -0.14293     -0.00100053    0.29969230   -
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  642   13     2.24602     6.72276    -1.84093     -0.00282119    0.84296226   -
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  643    8     3.71462     6.41101    -1.50200     -0.00401147    2.37803476   -
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  644   17     4.40852     5.47301    -3.40156     -0.00066380    0.23767782   -
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  645   17     5.40515     5.77192    -3.05682     -0.00149475    0.52607540   -
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  647   17     7.57658     4.50062    -2.91335     -0.00170037    0.52607540   -
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  650   17     5.93964     1.73798    -4.19757     -0.00147821    0.52607540   -
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  651   17     4.67857     2.09891    -4.40016     -0.00171367    0.52607540   -
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  652    8     4.59544     5.74105    -2.91394     -0.00140767    0.51899017   -
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  654    8     7.30048     5.10984    -2.43417     -0.00128444    0.51899017   -
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  657    8     6.59395     1.53816    -3.74046     -0.00114932    0.51899017   -
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  662   18     8.42897     1.14501    -0.93030     -0.00161864    0.56167009   -
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  670    8     8.26027     2.15936     1.01257     -0.00164519    0.54041647   -
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  671    8     7.25284     1.78352     2.14190     -0.00133711    0.54041647   -
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  672    8     5.99787     0.89635     2.40563     -0.00153047    0.54041647   -
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  673   19     4.21717     4.17469     2.93611     -0.00084689    0.24023875   -
0.00352520    0.16218315
  674   19     5.28760     3.90917     3.05626     -0.00165870    0.53339201   -
0.00310971    0.15776626
  675   19     6.56386     4.04497     2.66250     -0.00157248    0.53339201   -
0.00294808    0.15252742
  676   19     7.34882     4.67366     1.77318     -0.00169897    0.53339201   -
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  677   19     7.32461     5.54062     0.74843     -0.00177255    0.53339201   -
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  678   19     6.50102     6.29477     0.00327     -0.00168779    0.53339201   -
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  679   19     5.21159     6.63069    -0.16055     -0.00166072    0.53339201   -
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  685    8     5.90877     6.42848    -0.56184     -0.00125760    0.52300608   -
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  686    8     4.69952     6.58417    -0.52632     -0.00069035    0.29119849   -
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  692   12    -5.57818     1.18848    -2.20421     -0.00186611    0.95782110   -
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  693   12    -5.96321     0.95726    -1.08004     -0.00597510    1.91454418   -
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  694   10    -5.88336    -0.39118    -2.13387     -0.00463010    1.91454418   -
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  695   10    -6.15972    -0.63806    -0.98142     -0.00155884    0.95782110   -
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  696   16     0.71406    -4.91842     2.23975     -0.00037432    0.86794736   -
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  697   16     1.00522    -4.51676     2.75539     -0.00055797    0.86794736   -
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  698   11     2.28101    -4.09760     1.21203     -0.00349859    1.73180618   -
0.00202020    0.18058197
  699   18     6.04475    -1.18755     1.03917     -0.00223114    0.93959062   -
0.00237458    0.17768434
  700   18     6.39430    -1.35118    -0.11814     -0.00537787    1.87863113   -
0.00286265    0.17997939
  701   18     6.34942    -1.10362    -1.31189     -0.00176399    0.93959062   -
0.00187740    0.17606304
  702   11     5.14173    -2.30720     0.43161     -0.00676771    1.87863113   -
0.00360247    0.19103335
  703   11     5.33170    -2.25486    -1.03431     -0.00659378    1.87863113   -
0.00350989    0.19129080
  704   15    -5.56990     0.46425     2.83412     -0.00085708    0.89837409   -
0.00095403    0.14220062
  705   15    -6.02112    -0.08086     2.10117     -0.00206638    1.79335883   -
0.00115224    0.14507652
  706   12    -5.58616     1.68373     1.39870     -0.00369058    1.79335883   -
0.00205792    0.15875237
  707   12    -5.96236     1.11159     0.64432     -0.00175017    0.89837409   -
0.00194816    0.16193106
  708   19     4.03901     6.77678     0.22903     -0.00115698    0.82762736   -
0.00139794    0.16076255
  709   19     3.74026     6.54441     1.19182     -0.00353528    1.65359922   -
0.00213793    0.16346801
  710   13     2.42392     7.07709     0.22327     -0.00464524    1.65359922   -
0.00280917    0.16912138
  711   13     2.11309     6.76803     1.16032     -0.00145957    0.82762736   -
0.00176356    0.16537220];
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[MMIM] (Computation ID = 60)

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% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.49
%   total number of segments         =    606
%   number of charge corr segments   =    266
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N            -2.06335117619326    0.14364927569945    0.02185283794624   3.4582  -
0.0082     6.10    -0.00134    5.9148
% N             2.06335117619326   -0.14364927569945    0.02185283794624   3.4582  -
0.0081     6.10    -0.00133    5.9148
% C             0.00000000000000    0.00000000000000   -1.45823345708540   3.7795  -
0.0926    51.10    -0.00181    6.2361
% C            -1.29038020475695    0.09179542157490    2.52555561762947   3.7795  -
0.0405    52.63    -0.00077    6.2361
% C             1.29038020475695   -0.09179542157490    2.52555561762947   3.7795  -
0.0405    52.63    -0.00077    6.2361
% C            -4.69250247869296    0.33770235284020   -0.86752540275587   3.7795  -
0.0790    62.30    -0.00127    6.2361
% C             4.69250247869296   -0.33770235284020   -0.86752540275587   3.7795  -
0.0789    62.47    -0.00126    6.2361
% H             0.00000000000000    0.00000000000000   -3.50722253916853   2.4566  -
0.1003    25.04    -0.00401    4.9133
% H            -2.62799424020893    0.18608749208039    4.07734210182841   2.4566  -
0.0848    25.07    -0.00338    4.9133
% H             2.62799424020893   -0.18608749208039    4.07734210182841   2.4566  -
0.0848    25.07    -0.00338    4.9133
% H            -4.70798937721173    0.27728324864055   -2.93592748877725   2.4566  -
0.0651    23.00    -0.00283    4.9133
% H            -5.50846035609560    2.12972082656247   -0.21855036828485   2.4566  -
0.0634    25.11    -0.00253    4.9133
% H            -5.78689886323559   -1.25628285785357   -0.12001929945918   2.4566  -
0.0626    24.89    -0.00252    4.9133
% H             5.78689886323559    1.25628285785357   -0.12001929945918   2.4566  -
0.0626    24.88    -0.00252    4.9133
% H             4.70798937721173   -0.27728324864055   -2.93592748877725   2.4566  -
0.0652    22.79    -0.00286    4.9133
% H             5.50846035609560   -2.12972082656247   -0.21855036828485   2.4566  -
0.0634    25.11    -0.00253    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                  =       -305.383726
```

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%   Total energy + OC corr.      =       -305.379568
%   Dielectric energy            =         -0.086738      -2.360      -54.43
%   Diel. energy + OC corr.      =         -0.082579      -2.247      -51.82
%
%   Surface area of cavity [au]
acosmo =           514.271;
%   Total Volume of cavity [au]
vcosmo =           904.955;
%
%
% $screening_charge
%   cosmo           =   -1.02654
%   corrected total =   -0.99990
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1    -2.04346     3.60180     0.02515     -0.00011142    0.27778738   -
0.00040110    0.15917557
    2    1    -2.20037    -3.30868     0.16902     -0.00003653    0.13889369   -
0.00026302    0.15704044
    3    1    -2.62716    -3.26663     0.12750      0.00007158    0.41668107
0.00017179    0.15853219
    4    1    -1.72494     3.57988     0.21428     -0.00006635    0.13889369   -
0.00047770    0.15770209
    5    2     2.04359    -3.60177     0.02513     -0.00010161    0.27778738   -
0.00036577    0.15913225
    6    2     2.20028     3.30872     0.16909     -0.00003625    0.13889369   -
0.00026097    0.15703339
    7    2     2.62708     3.26667     0.12756      0.00007704    0.41668107
0.00018488    0.15850956
    8    2     1.72507    -3.57987     0.21426     -0.00006307    0.13889369   -
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    9    3    -0.35679    -3.63188    -0.47515     -0.00079327    0.66359074   -
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  483    6    -5.64395     1.78029     2.54376     -0.00075440    0.23092766   -
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  484    9    -5.01395     1.57225     3.27418     -0.00120462    0.23092766   -
0.00521642    0.17107587
  485   12    -5.70153     2.03555     2.40358     -0.00073743    0.23092766   -
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  486    6    -5.92991    -0.71786     2.59718     -0.00079122    0.25184851   -
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  487    9    -5.26819    -0.63842     3.32531     -0.00116878    0.25184851   -
0.00464080    0.17097123
  488   13    -6.02350    -0.97354     2.47766     -0.00074266    0.25184851   -
0.00294884    0.16534609
  489    9    -5.01278     1.09857     3.97221     -0.00396865    1.03225951   -
0.00384463    0.17318199
  490    9    -5.16112    -0.14194     3.99610     -0.00372220    1.03225951   -
0.00360588    0.17341923
  491    6    -5.90001     0.55264     2.79439     -0.00541449    2.89717833   -
0.00186889    0.16399739
  492   11    -4.17256    -1.85242    -4.03331     -0.00094644    0.24920184   -
0.00379787    0.17218338
  493   11    -5.31952    -1.76790    -4.02719     -0.00162897    0.55821625   -
0.00291817    0.16285853
  494   11    -6.44355    -0.95181    -4.04261     -0.00174165    0.55821625   -
0.00312003    0.15745914
  495   11    -6.81254     0.38692    -4.07895     -0.00193815    0.55821625   -
0.00347205    0.15660771
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0.00313320    0.16299032
  498   11    -3.89293     2.24602    -4.15512     -0.00082902    0.24920184   -
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0.00281279    0.16582503
  500    6    -6.09418    -1.64635    -3.69660     -0.00145067    0.53799680   -
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  501    6    -6.97853    -0.36999    -3.72726     -0.00160626    0.53799680   -
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  503    6    -5.82336     2.32291    -3.81457     -0.00146815    0.53799680   -
0.00272892    0.15573878
  504    6    -4.28890     2.56207    -3.83305     -0.00149078    0.53799680   -
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  508   12    -6.82315     3.42048    -1.76102     -0.00151418    0.53779774   -
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  509   12    -7.69983     2.74233    -0.99076     -0.00153010    0.53779774   -
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  515    6    -6.12323     3.51759    -2.20229     -0.00124786    0.52631383   -
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  518    6    -7.71589     1.68274     0.86167     -0.00134713    0.52631383   -
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  519    6    -6.67943     1.75823     1.95637     -0.00140577    0.52631383   -
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  520   13    -6.70348    -1.05798     2.15154     -0.00084706    0.23793692   -
0.00356000    0.16047831
  521   13    -7.53112    -0.80729     1.47438     -0.00141291    0.52699648   -
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  522   13    -8.13515    -0.94440     0.29765     -0.00140585    0.52699648   -
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  537   14     6.02345     0.97366     2.47766     -0.00076896    0.25181364   -
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  538    7     5.64394    -1.78033     2.54376     -0.00074863    0.23091896   -
0.00324196    0.16563913
  539   10     5.01394    -1.57230     3.27417     -0.00120362    0.23091896   -
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  541   10     5.01277    -1.09859     3.97220     -0.00396861    1.03235255   -
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  558    7     4.46325     3.36083    -0.39292     -0.00159509    0.51916720   -
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  559   15     4.17256     1.85244    -4.03330     -0.00086100    0.24921336   -
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  574   16     5.59362    -3.97721    -1.75254     -0.00164649    0.53779700   -
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  589   11    -3.35023    -0.78550    -4.90788     -0.00460543    1.64527300   -
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  590    8    -1.78684     1.08807    -5.08359     -0.00551007    1.64527300   -
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  591    8    -1.89129    -0.22881    -5.30509     -0.00601527    1.64527300   -
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  592    8    -1.90292    -1.25019    -4.90520     -0.00221260    0.82302955   -
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  593   15     3.19102    -1.55021    -4.72950     -0.00185068    0.82303493   -
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  594   15     3.29936    -0.53452    -5.12939     -0.00479592    1.64528361   -
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  601   13    -5.95071    -1.63402     2.55974     -0.00190428    1.22261014   -
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  602    9    -5.04551    -1.02631     3.88668     -0.00243799    1.22261014   -
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  603   14     5.95068     1.63405     2.55972     -0.00191516    1.22241276   -
0.00156671    0.16113775
  604   10     5.04548     1.02638     3.88667     -0.00244011    1.22241276   -
0.00199615    0.16754105
  605   16     5.69737    -2.45741     2.49247     -0.00075843    0.85739674   -
0.00088457    0.15991485
  606   10     4.71399    -1.94173     3.83424     -0.00122558    0.85739674   -
0.00142942    0.16613040];
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[EMMIM] (Computation ID = 62)

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% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.46
%   total number of segments         =    783
%   number of charge corr segments   =    324
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N            -1.48710880938996   -0.04371828769889   -0.50260883015266   3.4582  -
0.0032     3.65    -0.00087    5.9148
% N             1.83278607297673    2.40945263974423   -0.45303587526229   3.4582  -
0.0072     6.36    -0.00113    5.9148
% C             1.07688069792236   -0.04311038170174   -0.47651148937881   3.7795  -
0.0397    26.30    -0.00151    6.2361
% C            -3.15777282506718   -2.29402719499245   -0.42324886312666   3.7795  -
0.0362    27.35    -0.00132    6.2361
% C            -2.35132669456424    2.43124007080644   -0.48313494543185   3.7795  -
0.0251    48.09    -0.00052    6.2361
% C            -0.27928788483854    3.96491113304486   -0.46191999745057   3.7795  -
0.0323    52.81    -0.00061    6.2361
% C             2.74341553351509   -2.30007192808888   -0.53459628663139   3.7795  -
0.0502    49.57    -0.00101    6.2361
% C             4.44817100784135    3.33865332708418   -0.54787085865874   3.7795  -
0.0772    61.57    -0.00125    6.2361
% C            -3.90526750346047   -3.02729832058265    2.26500368624031   3.7795  -
0.0047    59.44    -0.00008    6.2361
% H            -2.17356811562281   -3.83399616827462   -1.39956892841999   2.4566  -
0.0526    19.90    -0.00265    4.9133
% H            -4.81805387472118   -1.82058298030066   -1.57215860752187   2.4566  -
0.0605    23.93    -0.00253    4.9133
% H            -4.35102559202855    2.88079879923383   -0.47662662094298   2.4566  -
0.0826    25.47    -0.00324    4.9133
% H            -0.11811015787056    6.00844253789348   -0.44599274694169   2.4566  -
0.0805    24.18    -0.00333    4.9133
% H             3.29092898286033   -2.79016652722690   -2.48399624367126   2.4566  -
0.0625    26.95    -0.00232    4.9133
% H             1.80179235543700   -3.94520406763037    0.30260934686563   2.4566  -
0.0461    17.52    -0.00263    4.9133
% H             4.48377484265411   -1.97095473739069    0.54533944063860   2.4566  -
0.0537    19.67    -0.00273    4.9133
% H             4.97162962689494    3.78831538762581   -2.50507714015041   2.4566  -
0.0601    25.23    -0.00238    4.9133
% H             5.73458835368825    1.90253942707116    0.20017430451365   2.4566  -
0.0504    17.82    -0.00283    4.9133
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% H             4.59157542596676    5.03974087134771    0.62466189282157   2.4566  -
0.0618    23.68    -0.00261    4.9133
% H            -5.17019044862672   -4.67407496026934    2.19457993359295   2.4566  -
0.0402    24.28    -0.00165    4.9133
% H            -4.91476144442668   -1.48422107663721    3.22120425511031   2.4566  -
0.0368    23.18    -0.00159    4.9133
% H            -2.24906954913994   -3.53666756305722    3.41277457395821   2.4566  -
0.0366    21.99    -0.00167    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                  =       -384.034735
%   Total energy + OC corr.       =       -384.030382
%   Dielectric energy             =         -0.080838      -2.200      -50.73
%   Diel. energy + OC corr.       =         -0.076485      -2.081      -48.00
%
%   Surface area of cavity [au]
acosmo =           628.940;
%   Total Volume of cavity [au]
vcosmo =          1194.956;
%
%
% $screening_charge
%   cosmo           =   -1.03108
%   corrected total =   -1.00020
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1    -1.72300    -0.25218    -3.94645      0.00008462    0.69446845
0.00012185    0.14786969
    2    1    -1.48360     0.21239    -3.95131     -0.00000029    0.13889369   -
0.00000210    0.14616844
    3    2     2.06374     2.57677     2.99340      0.00016622    0.55557476
0.00029918    0.14782367
    4    2     1.69588     2.48663    -3.90764     -0.00012071    0.13889369   -
0.00086906    0.15353409
    5    2     2.06249     2.33871    -3.90285     -0.00004159    0.13889369   -
0.00029947    0.15577002
    6    2     1.60331     2.48020     2.99683     -0.00003477    0.13889369   -
0.00025036    0.14650485
    7    3     2.30894     0.12190     3.09268     -0.00092032    0.66359074   -
0.00138688    0.15649489
    8    3     0.03670    -0.15227    -4.10836     -0.00042913    0.66359074   -
0.00064668    0.15368732
    9    3     2.15076     0.45582    -4.06566     -0.00096049    0.66359074   -
0.00144742    0.16023752
   10    3     1.49708    -0.28918     3.27145     -0.00109785    0.82948843   -
0.00132353    0.15359301
   11    3     1.56539     0.66763     3.20324     -0.00086704    0.99538612   -
0.00087106    0.15188217
   12    3     1.41660     0.85432    -4.13210     -0.00071830    0.66359074   -
0.00108244    0.15594417
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   13    3     0.51502     0.53846    -4.16843     -0.00136245    0.99538612   -
0.00136876    0.15334175
   14    3     0.52140    -0.77373    -4.14282     -0.00122748    0.99538612   -
0.00123317    0.15721790
   15    3     1.41009     0.01409    -4.24080     -0.00102092    0.82948843   -
0.00123079    0.15716988
   16    3     0.72817     0.47927     3.25040     -0.00161540    0.99538612   -
0.00162289    0.15036647
   17    4    -5.05566    -5.33431    -1.62290     -0.00079681    0.99538612   -
0.00080050    0.13638607
   18    4    -3.76593    -2.75090    -4.12538     -0.00062751    1.32718149   -
0.00047281    0.14255245
   19    4    -3.29608    -3.65680    -3.94576     -0.00038418    0.99538612   -
0.00038596    0.14343837
   20    4    -4.45968    -5.31273    -2.28790     -0.00080435    0.99538612   -
0.00080808    0.13912546
   21    4    -4.26015    -5.79696    -1.31695     -0.00064393    0.66359074   -
0.00097037    0.14032817
   22    4    -5.27342    -4.50593    -2.64045     -0.00069857    1.16128380   -
0.00060155    0.13737037
   23    4    -4.37428    -3.82650    -3.65683     -0.00027093    1.16128380   -
0.00023330    0.13905999
   24    4    -2.88070    -2.36555    -4.19186     -0.00051263    1.16128380   -
0.00044144    0.14551562
   25    4    -1.99365    -2.05204    -4.01080     -0.00079236    0.66359074   -
0.00119405    0.15202516
   26    4    -5.85611    -4.60445    -1.71375     -0.00095797    1.16128380   -
0.00082493    0.13710564
   27    4    -3.61547    -1.33708    -4.05079     -0.00069156    0.66359074   -
0.00104215    0.14929610
   28    4    -1.99283    -2.78793    -3.98461     -0.00097238    0.82948843   -
0.00117226    0.15296925
   29    4    -4.38615    -4.65298    -3.10856     -0.00043260    0.99538612   -
0.00043460    0.13846435
   30    4    -3.72190    -6.01348    -0.78639     -0.00041916    0.33179537   -
0.00126332    0.14355301
   31    4    -6.40267    -4.05551    -1.23083     -0.00037998    0.49769306   -
0.00076347    0.13968418
   32    4    -2.96798    -1.31392    -4.06847     -0.00045918    0.66359074   -
0.00069196    0.14857670
   33    5    -3.71395     4.86814     2.06420      0.00043545    1.16128380
0.00037498    0.13143214
   34    5    -4.18521     5.39268    -1.94975     -0.00103078    0.99538612   -
0.00103556    0.14278818
   35    5    -3.91222     2.77288    -3.90822      0.00029001    1.49307918
0.00019424    0.12994374
   36    5    -4.88072     2.77675    -3.27009     -0.00113526    1.32718149   -
0.00085539    0.14200480
   37    5    -4.25279     5.66005    -0.97653     -0.00070559    0.66359074   -
0.00106329    0.14929769
   38    5    -4.51317     4.46172     1.85944     -0.00085030    0.99538612   -
0.00085424    0.13916605
   39    5    -3.97665     3.73922     2.66831      0.00026221    1.16128380
0.00022579    0.12927625
   40    5    -4.15268     5.31793     1.16194     -0.00044139    0.82948843   -
0.00053213    0.14191481
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   41    5    -4.07374     5.77105    -0.07927     -0.00062497    0.33179537   -
0.00188360    0.14898174
   42    5    -3.90119     4.99299    -2.78956     -0.00006155    1.16128380   -
0.00005300    0.13352026
   43    5    -4.24497     3.81830    -3.44531      0.00022002    1.16128380
0.00018946    0.13106907
   44    5    -4.49050     1.80096    -3.53453      0.00003788    0.82948843
0.00004567    0.14248465
   45    5    -1.80431     2.13172     3.24449      0.00034333    0.66359074
0.00051739    0.13029936
   46    5    -2.17636     2.92972     3.25919      0.00097544    0.82948843
0.00117596    0.12409330
   47    5    -3.03004     3.93128     2.91883      0.00126755    1.16128380
0.00109151    0.12272711
   48    5    -2.72004     3.11398    -4.18209      0.00191184    1.65897686
0.00115242    0.12291498
   49    5    -3.39010     1.83914    -4.06848     -0.00006211    1.32718149   -
0.00004680    0.13344794
   50    5    -2.74810     1.36988    -4.08875     -0.00001276    0.82948843   -
0.00001538    0.13607994
   51    5    -4.59854     4.39456    -2.80254     -0.00072094    0.82948843   -
0.00086914    0.13919137
   52    5    -4.32392     5.52705     0.41629     -0.00110592    0.49769306   -
0.00222209    0.14829862
   53    5    -4.67247     3.35689     2.35227     -0.00057360    0.82948843   -
0.00069151    0.13865858
   54    5    -1.89443     2.04597    -4.21505      0.00087184    1.49307918
0.00058392    0.13091363
   55    5    -3.12647     2.95491     3.17870      0.00080874    1.32718149
0.00060937    0.12567239
   56    5    -3.34231     4.16052    -3.69434      0.00125899    1.16128380
0.00108413    0.12367006
   57    6     0.96905     5.36312    -3.74384     -0.00008063    0.49769306   -
0.00016201    0.14050290
   58    6    -2.22674     6.01601    -2.96884      0.00039354    1.16128380
0.00033889    0.13116538
   59    6    -2.55416     6.57423     1.05486     -0.00109093    0.99538612   -
0.00109599    0.14302416
   60    6    -0.11516     5.51701     2.98023      0.00021743    1.49307918
0.00014562    0.13098729
   61    6     0.05792     6.43852     2.37566     -0.00080580    1.16128380   -
0.00069389    0.14203835
   62    6    -2.79799     6.72911     0.08545     -0.00058617    0.66359074   -
0.00088333    0.14936886
   63    6    -1.60064     6.65715    -2.76196     -0.00076756    0.99538612   -
0.00077112    0.13870194
   64    6     1.03772     6.36480    -3.06776     -0.00128559    0.99538612   -
0.00129155    0.14922218
   65    6     0.34356     5.85201    -3.67677     -0.00016258    0.99538612   -
0.00016333    0.13645101
   66    6    -1.07584     5.94070    -3.58379      0.00043955    1.16128380
0.00037850    0.12864447
   67    6    -2.51911     6.55742    -2.05765     -0.00046359    0.82948843   -
0.00055889    0.14173688
   68    6    -2.96464     6.60132    -0.81197     -0.00067427    0.33179537   -
0.00203218    0.14904051
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   69    6    -2.35843     6.13878     1.82625     -0.00004861    1.16128380   -
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   70    6    -1.01958     6.14899     2.53242      0.00013157    1.16128380
0.00011330    0.13184837
   71    6     0.98096     5.78684     2.60022     -0.00008033    0.82948843   -
0.00009684    0.14400512
   72    6     0.55970     4.61788    -4.08877      0.00028016    1.32718149
0.00021110    0.13489407
   73    6     0.13343     3.40979    -4.17753      0.00048256    1.65897686
0.00029088    0.13447884
   74    6    -0.80822     4.12775    -4.20063      0.00151392    1.16128380
0.00130366    0.12397822
   75    6    -1.60555     5.09536    -3.81563      0.00134113    1.32718149
0.00101051    0.12247054
   76    6    -0.79082     4.47558     3.24777      0.00187598    1.65897686
0.00113081    0.12355871
   77    6     0.62404     4.74062     3.12508     -0.00015073    1.32718149   -
0.00011357    0.13464759
   78    6     0.77873     3.93005     3.16626      0.00005698    0.66359074
0.00008586    0.13604486
   79    6    -1.47119     6.66443     1.89949     -0.00074468    0.82948843   -
0.00089776    0.13981266
   80    6    -2.66190     6.77406    -1.30816     -0.00109707    0.49769306   -
0.00220432    0.14831875
   81    6    -0.32513     6.46335    -3.29741     -0.00064975    1.16128380   -
0.00055951    0.13837799
   82    6     1.01683     6.54798     1.97369     -0.00060714    0.33179537   -
0.00182988    0.15477068
   83    6    -0.01409     3.37111     3.26116      0.00071473    1.49307918
0.00047869    0.13141610
   84    6    -0.46011     5.05906    -4.07501      0.00055376    1.16128380
0.00047685    0.12654155
   85    6    -1.64251     5.46778     2.72670      0.00135343    1.32718149
0.00101978    0.12482609
   86    7     2.43108    -1.93364     3.21408     -0.00048152    0.49769306   -
0.00096750    0.15138027
   87    7     6.35923    -2.22053    -1.63177     -0.00036680    0.82948843   -
0.00044220    0.14784731
   88    7     4.58569    -5.58423    -0.85778     -0.00041735    1.32718149   -
0.00031447    0.13382355
   89    7     3.30110    -2.00490     3.19183     -0.00055503    1.16128380   -
0.00047795    0.15089784
   90    7     3.72585    -2.99508     3.04816     -0.00006297    0.66359074   -
0.00009490    0.14612314
   91    7     2.69250    -2.76475     3.21585     -0.00007247    0.66359074   -
0.00010920    0.14688186
   92    7     1.76719    -5.07629    -2.90602      0.00013730    0.82948843
0.00016553    0.14894365
   93    7     4.55641    -5.29649    -1.95539     -0.00083850    1.49307918   -
0.00056159    0.13770640
   94    7     6.10704    -2.43353    -2.25286     -0.00013883    0.66359074   -
0.00020921    0.14583431
   95    7     4.23674    -4.22400     2.35552     -0.00027530    1.32718149   -
0.00020743    0.14115285
   96    7     3.57642    -4.51785     2.41021     -0.00016466    0.82948843   -
0.00019851    0.14225216
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   97    7     5.90889    -1.65374    -2.49577     -0.00012399    0.66359074   -
0.00018685    0.15053096
   98    7     6.25708    -3.32061    -1.48160     -0.00043174    1.65897686   -
0.00026025    0.14150676
   99    7     5.57621    -4.72121    -1.16510     -0.00045506    1.49307918   -
0.00030478    0.13506505
  100    7     3.43928    -5.94815    -1.23560     -0.00066883    1.49307918   -
0.00044795    0.13807461
  101    7     2.11787    -5.72225    -2.01159     -0.00035302    1.32718149   -
0.00026599    0.14462288
  102    7     5.14774    -4.66585     1.17027     -0.00075290    1.32718149   -
0.00056729    0.13912488
  103    7     5.03826    -5.22898     0.12824     -0.00049518    1.65897686   -
0.00029848    0.13430941
  104    7     3.92437    -5.85155    -0.00874     -0.00068191    0.99538612   -
0.00068507    0.13813561
  105    7     3.38466    -1.07981     2.98452     -0.00042181    0.49769306   -
0.00084753    0.15891698
  106    7     3.03312    -3.60893     2.99914     -0.00035946    1.32718149   -
0.00027085    0.14440625
  107    7     0.95417    -2.86345    -3.81565     -0.00035068    0.16589769   -
0.00211383    0.16384102
  108    7     3.17653    -5.68368    -2.16178     -0.00022142    1.16128380   -
0.00019067    0.14000958
  109    7     5.75870    -4.12424    -1.90010     -0.00049407    0.99538612   -
0.00049636    0.13909593
  110    7     4.23848    -5.28293     1.24066     -0.00044774    1.49307918   -
0.00029988    0.13816084
  111    7     5.89774    -4.36247    -0.25001     -0.00088145    1.16128380   -
0.00075903    0.13867019
  112    8     3.88255     2.53267     3.10108     -0.00071785    0.82948843   -
0.00086542    0.15114441
  113    8     5.36928     6.88445    -1.47685     -0.00017390    0.99538612   -
0.00017471    0.14082584
  114    8     8.11915     4.08576    -1.04768     -0.00118043    1.32718149   -
0.00088943    0.13640208
  115    8     6.74203     1.09993    -2.55049     -0.00029749    0.82948843   -
0.00035865    0.14898756
  116    8     3.45284     3.55972     3.09147     -0.00061204    0.66359074   -
0.00092232    0.15041553
  117    8     4.51725     3.38854     3.23063     -0.00060133    1.16128380   -
0.00051781    0.14621877
  118    8     5.49311     3.75148     3.06073     -0.00028455    1.16128380   -
0.00024503    0.14339002
  119    8     4.68030     2.15590     3.03425     -0.00117801    1.16128380   -
0.00101440    0.15228919
  120    8     5.37644     2.39437     2.99204     -0.00055332    0.82948843   -
0.00066706    0.14972098
  121    8     4.06741     1.72806    -3.94570     -0.00074956    0.33179537   -
0.00225910    0.16342984
  122    8     6.80839     1.70707    -3.00785     -0.00027708    0.66359074   -
0.00041755    0.14665839
  123    8     7.77515     4.19379    -2.12396     -0.00145363    1.49307918   -
0.00097358    0.13908386
  124    8     5.29349     6.56877    -2.31872     -0.00021049    0.99538612   -
0.00021146    0.14132822
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  125    8     6.94349     4.22598     2.14847     -0.00051055    1.49307918   -
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  126    8     6.97758     3.31791     2.26031     -0.00043189    0.82948843   -
0.00052067    0.14320138
  127    8     4.25628     6.80314    -2.04610     -0.00029017    1.16128380   -
0.00024987    0.14486999
  128    8     6.44949     6.46022    -1.27909     -0.00090120    1.49307918   -
0.00060359    0.13778658
  129    8     7.59190     5.30694    -1.27377     -0.00127820    1.49307918   -
0.00085609    0.13560169
  130    8     8.08520     3.08332    -1.54332     -0.00084938    1.32718149   -
0.00063998    0.13918327
  131    8     7.40989     1.72907    -2.25715     -0.00032873    1.16128380   -
0.00028308    0.14475831
  132    8     5.90946     1.27733    -3.35852     -0.00043053    0.66359074   -
0.00064879    0.15257926
  133    8     4.35436     7.04413    -1.28602     -0.00046613    0.66359074   -
0.00070244    0.14763893
  134    8     7.50673     4.89937     1.03123     -0.00129598    1.49307918   -
0.00086799    0.13844662
  135    8     7.97888     4.58364    -0.02998     -0.00141371    1.65897686   -
0.00085216    0.13607574
  136    8     8.21363     3.26760    -0.23106     -0.00137966    1.16128380   -
0.00118805    0.14157434
  137    8     3.91781     4.03312     3.12919     -0.00037050    0.49769306   -
0.00074444    0.15036698
  138    8     6.13467     3.16967     2.83021     -0.00026045    1.16128380   -
0.00022428    0.14344544
  139    8     5.27725     1.39312    -3.68024     -0.00010893    0.16589769   -
0.00065659    0.15732176
  140    8     7.66474     2.68176    -2.42038     -0.00045963    0.99538612   -
0.00046176    0.14125897
  141    8     6.91800     5.82661    -1.96000     -0.00106275    1.32718149   -
0.00080075    0.13803622
  142    8     3.80108     6.39493    -2.67499     -0.00053396    0.82948843   -
0.00064372    0.14896922
  143    8     7.84360     3.75981     1.05770     -0.00128709    1.49307918   -
0.00086204    0.14008872
  144    8     7.32101     5.77245    -0.21987     -0.00192250    1.65897686   -
0.00115885    0.13794892
  145    8     7.90433     2.16785    -1.53190     -0.00064742    0.66359074   -
0.00097563    0.14477707
  146    9    -2.78481    -6.32478     3.73316      0.00063605    0.82948843
0.00076679    0.11413754
  147    9    -5.50227    -3.90945     5.57494      0.00054020    1.32718149
0.00040703    0.10118383
  148    9    -7.61298    -2.53156     2.80485      0.00098158    1.32718149
0.00073960    0.11206073
  149    9    -1.78236    -1.06438     4.69899      0.00025260    0.66359074
0.00038066    0.12754251
  150    9    -7.63240    -3.47237     2.70629      0.00054374    0.99538612
0.00054626    0.11092445
  151    9    -5.98501    -4.71191     4.93353      0.00028662    1.49307918
0.00019197    0.10365421
  152    9    -3.54893    -6.60946     3.41630      0.00058176    0.99538612
0.00058446    0.11247979
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  153    9    -3.69433    -6.49077     0.76691     -0.00007403    0.66359074   -
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  154    9    -2.80234    -1.67203     5.61626      0.00103818    1.32718149
0.00078224    0.11533683
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0.00287101    0.16546276];
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[BMIM] Computation ID = 63)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.44
%   total number of segments         =    921
%   number of charge corr segments   =    363
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N             0.36335864061363    1.15109508808802   -1.57527003043041   3.4582  -
0.0038     3.69    -0.00103    5.9148
% N             3.68752960281486    3.61953949450009   -1.54858624338930   3.4582  -
0.0081     6.23    -0.00130    5.9148
% C            -1.22918283849876   -1.15500780730144   -1.46804834392917   3.7795  -
0.0300    21.87    -0.00137    6.2361
% C            -1.93852834004166   -1.90247467648507    1.23651659535903   3.7795  -
0.0081    22.59    -0.00036    6.2361
% C            -3.57320115539639   -4.30170378176081    1.28763452796823   3.7795
0.0085    26.02     0.00033    6.2361
% C             2.90566635822330    1.19687804794635   -1.59017207239114   3.7795  -
0.0765    46.99    -0.00163    6.2361
% C            -0.50204621744455    3.62246013803586   -1.51714302992429   3.7795  -
0.0337    48.32    -0.00070    6.2361
% C             1.57451632072437    5.16713834850577   -1.50776276203162   3.7795  -
0.0416    52.88    -0.00079    6.2361
% C            -4.31606175667911   -5.07775353715213    3.97584018756085   3.7795
0.0454    58.31     0.00078    6.2361
% C             6.33222626101797    4.47326343948446   -1.65468148493442   3.7795  -
0.0807    63.32    -0.00127    6.2361
% H            -0.16886077899105   -2.66411304407593   -2.41941415622276   2.4566  -
0.0608    24.25    -0.00251    4.9133
% H            -2.90978853135449   -0.76395779271906   -2.62043661302732   2.4566  -
0.0598    24.89    -0.00240    4.9133
% H            -2.95949108555224   -0.33117667454926    2.14727284896147   2.4566  -
0.0324    24.01    -0.00135    4.9133
% H            -0.19815687429448   -2.20346676523962    2.34274021204694   2.4566  -
0.0330    24.47    -0.00135    4.9133
% H            -2.54012415615536   -5.86178777281540    0.36848392194595   2.4566  -
0.0259    25.13    -0.00103    4.9133
% H            -5.29111718890370   -3.99103145376796    0.14877994825397   2.4566  -
0.0258    25.19    -0.00102    4.9133
% H             4.12881198843947   -0.44639336709698   -1.63706978924951   2.4566  -
0.1092    27.61    -0.00396    4.9133
% H            -2.50150724752261    4.07300631639370   -1.48561988104420   2.4566  -
0.0855    26.01    -0.00329    4.9133
```

```
% H             1.72457128601654    7.21211589083798   -1.48896399141759   2.4566  -
0.0842    24.59    -0.00342    4.9133
% H            -5.46557635705350   -6.80801821468008    3.95091338850226   2.4566  -
0.0239    24.29    -0.00098    4.9133
% H            -5.43203912862076   -3.59403281378042    4.91582461970980   2.4566  -
0.0215    25.09    -0.00086    4.9133
% H            -2.64039719497308   -5.45302122054270    5.15120351256064   2.4566  -
0.0215    24.97    -0.00086    4.9133
% H             6.77839480754904    5.13068067117905   -3.57123056773933   2.4566  -
0.0623    25.17    -0.00247    4.9133
% H             7.57178348421803    2.89474778357179   -1.14686812767788   2.4566  -
0.0636    23.33    -0.00273    4.9133
% H             6.59922010186460    6.01301370342383   -0.29394266946009   2.4566  -
0.0627    24.51    -0.00256    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                =       -423.345346
%   Total energy + OC corr.     =       -423.340913
%   Dielectric energy           =         -0.083719      -2.278      -52.54
%   Diel. energy + OC corr.     =         -0.079287      -2.157      -49.75
%
%   Surface area of cavity [au]
acosmo =           723.732;
%   Total Volume of cavity [au]
vcosmo =          1353.716;
%
%
% $screening_charge
%   cosmo           =   -1.03611
%   corrected total =   -1.00037
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]           charge       area [au]
charge/area    potential [au]
%
data = [1    1     0.07536     0.97201    -5.01680      0.00003417    0.69446845
0.00004920    0.15104575
    2    1     0.30639     1.44081    -5.02084     -0.00004064    0.13889369   -
0.00029260    0.14989940
    3    2     3.97134     3.74145     1.89581      0.00004597    0.55557476
0.00008274    0.15370278
    4    2     3.50081     3.74097    -4.99959     -0.00014693    0.13889369   -
0.00105785    0.15747159
    5    2     3.86549     3.58830    -5.00204     -0.00010876    0.13889369   -
0.00078305    0.15920493
    6    2     3.50979     3.65079     1.90492     -0.00007464    0.13889369   -
0.00053738    0.15255242
    7    3    -1.71290    -1.63793    -5.18517     -0.00050581    1.16128380   -
0.00043556    0.14317188
    8    3    -1.28841    -2.57335    -4.97076     -0.00022414    0.99538612   -
0.00022518    0.14375312
    9    3    -2.27724    -4.06408    -3.64133     -0.00038942    0.49769306   -
0.00078245    0.13780324
```

```
   10    3    -2.99635    -3.49478    -3.85277     -0.00073569    1.16128380   -
0.00063351    0.13566260
   11    3    -2.41488    -2.63078    -4.73920     -0.00052834    1.16128380   -
0.00045496    0.13935105
   12    3    -0.93195    -1.26796    -5.23409     -0.00059314    1.16128380   -
0.00051076    0.14656860
   13    3    -0.06115    -0.91120    -5.05419     -0.00067360    0.66359074   -
0.00101508    0.15372469
   14    3    -1.71405    -0.27262    -5.11091     -0.00067891    0.66359074   -
0.00102309    0.15077138
   15    3    -0.02649    -1.64581    -5.01724     -0.00088472    0.82948843   -
0.00106658    0.15413561
   16    3    -2.13263    -3.41446    -4.35992     -0.00016804    0.66359074   -
0.00025323    0.13846345
   17    3    -1.06824    -0.21982    -5.12642     -0.00037404    0.66359074   -
0.00056365    0.15047137
   18    4    -0.13383     0.42167     3.60833      0.00056695    1.16128380
0.00048821    0.12750361
   19    4     0.90430    -4.36351     0.85453     -0.00009159    0.33179537   -
0.00027606    0.14028513
   20    4    -0.91547     0.67603     3.80338      0.00049163    0.82948843
0.00059269    0.12394929
   21    4    -2.41631    -0.66709     4.77625      0.00003012    0.16589769
0.00018154    0.11092377
   22    4    -5.07655    -0.00586     0.32003     -0.00037048    0.49769306   -
0.00074439    0.13784588
   23    4    -1.21749    -0.97588     4.82896      0.00075162    0.82948843
0.00090613    0.11068195
   24    4    -0.81344    -0.19778     4.41650      0.00109182    1.16128380
0.00094019    0.11665537
   25    4     1.14911    -4.05205     0.87581     -0.00015565    0.16589769   -
0.00093825    0.14538175
   26    4    -1.74439    -0.30150     4.65460      0.00042194    0.49769306
0.00084780    0.11306276
   27    4    -5.30411    -0.26104     0.72384      0.00003936    0.16589769
0.00023726    0.13173234
   28    5    -5.46430    -7.39867     0.23083      0.00095071    0.99538612
0.00095512    0.08475568
   29    5    -4.35010    -5.25688    -2.28566      0.00122942    1.16128380
0.00105867    0.10706484
   30    5    -6.34354    -1.78533     1.81414      0.00021668    0.49769306
0.00043537    0.10803381
   31    5    -6.79567    -2.35333     1.60966      0.00010823    0.16589769
0.00065238    0.10421485
   32    5    -3.75254    -5.88475    -2.13964      0.00118020    0.99538612
0.00118567    0.10582592
   33    5    -4.54531    -7.71112    -0.02202      0.00062479    0.99538612
0.00062768    0.08907620
   34    5    -0.17120    -5.86247     1.81178      0.00018514    0.66359074
0.00027900    0.11542663
   35    5    -5.46381    -6.90503    -0.69544      0.00135061    1.32718149
0.00101765    0.08778949
   36    5    -4.85674    -6.15298    -1.74710      0.00127423    0.99538612
0.00128014    0.09588811
   37    5    -6.21186    -6.65458    -0.04867      0.00063379    0.82948843
0.00076407    0.08739214
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   38    5    -6.36422    -1.75330     1.29135      0.00005915    0.16589769
0.00035657    0.11171519
   39    5    -4.76789    -6.87619    -1.20818      0.00112928    0.99538612
0.00113452    0.09140068
   40    5    -0.47423    -6.29863     2.12009      0.00009635    0.16589769
0.00058078    0.10903460
   41    6     2.51042     2.04181     2.07236     -0.00128090    0.82948843   -
0.00154420    0.15401397
   42    6     5.08997     0.56067     1.42783     -0.00132503    0.99538612   -
0.00133117    0.16743946
   43    6     3.93927     0.01975    -5.02969     -0.00124329    1.32718149   -
0.00093679    0.16066149
   44    6     4.55429    -0.56369    -4.49993     -0.00172956    0.99538612   -
0.00173758    0.17055421
   45    6     5.32089    -0.25913     0.92598     -0.00166328    0.82948843   -
0.00200519    0.17678067
   46    6     4.50558     0.03201     1.62971     -0.00100646    0.99538612   -
0.00101113    0.16401339
   47    6     4.13285    -0.57347     1.51533     -0.00065987    0.49769306   -
0.00132585    0.16614669
   48    6     3.20944    -0.84212    -4.75789     -0.00123912    1.16128380   -
0.00106703    0.16493741
   49    6     5.02733     0.40434    -4.61585     -0.00072452    0.99538612   -
0.00072788    0.16742294
   50    6     4.25398     1.52825     1.92502     -0.00089775    1.16128380   -
0.00077307    0.15847097
   51    6     3.17936     1.64120     2.15308     -0.00087931    0.99538612   -
0.00088339    0.15407504
   52    6     2.02066     1.23888    -5.26430     -0.00089511    1.16128380   -
0.00077079    0.15356644
   53    6     2.91524     0.54021    -5.31213     -0.00113144    1.49307918   -
0.00075779    0.15537457
   54    6     3.98841     1.27797    -5.21031     -0.00183767    1.82487455   -
0.00100701    0.15807475
   55    6     3.66817    -1.37622    -4.25137     -0.00190268    0.99538612   -
0.00191150    0.17510880
   56    6     4.39871    -1.01908     1.08277     -0.00114298    0.49769306   -
0.00229656    0.17440922
   57    6     5.50785    -0.05627    -4.02791     -0.00133018    0.66359074   -
0.00200452    0.17821928
   58    6     2.78447     1.99633    -5.28212     -0.00154036    1.49307918   -
0.00103167    0.15467941
   59    6     3.76209     0.69796     2.05700     -0.00116985    1.16128380   -
0.00100738    0.15717367
   60    6     2.28755    -0.15867    -5.06359     -0.00099371    0.99538612   -
0.00099832    0.15875796
   61    7    -1.83542     6.04238     1.06172      0.00021180    1.16128380
0.00018239    0.13734313
   62    7    -2.35023     6.59485    -2.94312     -0.00110085    0.99538612   -
0.00110595    0.14848082
   63    7    -2.10011     3.98851    -4.92249      0.00004250    1.49307918
0.00002846    0.13490322
   64    7    -3.01957     4.08441    -4.29795     -0.00089850    1.16128380   -
0.00077372    0.14560028
   65    7    -2.40702     6.85552    -1.96740     -0.00087473    0.66359074   -
0.00131818    0.15497285
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   66    7    -2.63705     5.63777     0.86292     -0.00099454    0.99538612   -
0.00099915    0.14465495
   67    7    -2.09212     4.90944     1.66087      0.00004790    1.16128380
0.00004125    0.13460922
   68    7    -2.28373     6.49861     0.16743     -0.00063265    0.82948843   -
0.00076270    0.14768083
   69    7    -2.21812     6.96024    -1.07141     -0.00063821    0.33179537   -
0.00192350    0.15475278
   70    7    -2.07563     6.20083    -3.78873     -0.00033023    1.16128380   -
0.00028437    0.13930694
   71    7    -2.42720     5.03086    -4.44876     -0.00003826    1.16128380   -
0.00003295    0.13635813
   72    7    -2.67480     3.01430    -4.54921     -0.00015098    0.82948843   -
0.00018201    0.14665858
   73    7     0.08550     3.29697     2.20216      0.00018630    0.66359074
0.00028074    0.13584243
   74    7    -0.28593     4.09503     2.22644      0.00080360    0.82948843
0.00096879    0.12979277
   75    7    -1.14273     5.09932     1.90234      0.00108799    1.16128380
0.00093688    0.12854937
   76    7    -0.91080     4.33092    -5.20702      0.00159404    1.65897686
0.00096085    0.12850708
   77    7    -1.58029     3.05564    -5.09488     -0.00024881    1.32718149   -
0.00018748    0.13811626
   78    7    -0.93880     2.58623    -5.12541     -0.00016047    0.82948843   -
0.00019345    0.14081077
   79    7    -2.77341     5.60283    -3.79821     -0.00070145    0.82948843   -
0.00084565    0.14456247
   80    7    -2.46299     6.71295    -0.57484     -0.00112092    0.49769306   -
0.00225223    0.15399981
   81    7    -2.79157     4.52964     1.34983     -0.00072817    0.82948843   -
0.00087786    0.14357533
   82    7    -3.40007     3.19343    -3.90494     -0.00075595    0.33179537   -
0.00227835    0.15724581
   83    7    -0.08619     3.26277    -5.25637      0.00055786    1.49307918
0.00037363    0.13627556
   84    7    -1.23685     4.12122     2.15651      0.00060062    1.32718149
0.00045256    0.13088790
   85    7    -1.52713     5.37437    -4.70528      0.00105868    1.16128380
0.00091165    0.12945056
   86    8    -0.40211     7.21225    -3.99668      0.00019800    1.16128380
0.00017050    0.13709854
   87    8    -0.70378     7.76097     0.03034     -0.00125928    0.99538612   -
0.00126511    0.14899309
   88    8     1.75472     6.71352     1.93615      0.00004377    1.49307918
0.00002932    0.13633647
   89    8     1.91840     7.63712     1.33216     -0.00088030    1.16128380   -
0.00075804    0.14707737
   90    8    -0.95539     7.91635    -0.93700     -0.00061750    0.66359074   -
0.00093054    0.15523407
   91    8     0.22192     7.85642    -3.79303     -0.00094274    0.99538612   -
0.00094711    0.14444574
   92    8     2.85960     7.57920    -4.11826     -0.00154080    0.99538612   -
0.00154794    0.15480670
   93    8     2.29794     6.96147    -4.75448     -0.00053116    1.32718149   -
0.00040021    0.14275829
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   94    8     0.74476     7.14444    -4.61999      0.00026922    1.16128380
0.00023183    0.13448047
   95    8    -0.69092     7.75030    -3.08237     -0.00049018    0.82948843   -
0.00059094    0.14749607
   96    8    -1.12775     7.78935    -1.83345     -0.00074648    0.33179537   -
0.00224983    0.15489333
   97    8    -0.50013     7.32513     0.79946     -0.00025969    1.16128380   -
0.00022362    0.14032572
   98    8     0.84366     7.34136     1.49606     -0.00006176    1.16128380   -
0.00005318    0.13746102
   99    8     2.84659     6.99010     1.54885     -0.00009455    0.82948843   -
0.00011399    0.14880404
  100    8     2.38387     5.83162    -5.13923     -0.00012561    1.32718149   -
0.00009464    0.14078842
  101    8     1.94217     4.68577    -5.23835      0.00017252    1.49307918
0.00011555    0.13979642
  102    8     1.01790     5.33418    -5.24226      0.00122786    1.16128380
0.00105733    0.13018137
  103    8     0.28233     6.29769    -4.87471      0.00106785    1.16128380
0.00091954    0.12856849
  104    8     1.08672     5.66787     2.20649      0.00160620    1.65897686
0.00096819    0.12934813
  105    8     2.49919     5.94094     2.07421     -0.00023217    1.32718149   -
0.00017493    0.14001025
  106    8     2.76222     5.19023     2.08015     -0.00018252    0.82948843   -
0.00022003    0.14278322
  107    8     0.38471     7.85551     0.86738     -0.00085591    0.82948843   -
0.00103186    0.14548785
  108    8    -0.82952     7.96471    -2.33146     -0.00116074    0.49769306   -
0.00233224    0.15406550
  109    8     1.49461     7.67068    -4.33797     -0.00081725    1.16128380   -
0.00070375    0.14403872
  110    8     2.87380     7.75263     0.92356     -0.00056628    0.33179537   -
0.00170672    0.15913434
  111    8     1.86959     4.56767     2.21217      0.00050496    1.49307918
0.00033820    0.13712091
  112    8     1.36178     6.26715    -5.11732      0.00036892    1.16128380
0.00031768    0.13247929
  113    8     0.22589     6.65636     1.69346      0.00109424    1.32718149
0.00082448    0.13084323
  114    9    -2.95873    -8.26063     5.49613      0.00126829    0.82948843
0.00152901    0.07042970
  115    9    -5.81832    -6.00002     7.31903      0.00127477    1.32718149
0.00096051    0.06323880
  116    9    -8.05863    -4.70328     4.34631      0.00195644    1.49307918
0.00131034    0.07208672
  117    9    -2.31041    -2.92559     6.34853      0.00081323    0.66359074
0.00122550    0.08863792
  118    9    -7.26220    -6.40542     2.01575      0.00013700    0.33179537
0.00041291    0.08245335
  119    9    -7.99970    -5.76756     4.46505      0.00125976    0.99538612
0.00126560    0.06969084
  120    9    -6.25080    -6.84639     6.69853      0.00124930    1.49307918
0.00083673    0.06474383
  121    9    -3.58435    -8.62299     5.06225      0.00165184    1.32718149
0.00124462    0.06990084
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  910   22    -0.68727    -3.79577     5.76376     -0.00068048    1.72027151   -
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  911   14     0.68208    -4.26218     3.72959     -0.00130202    1.72027151   -
0.00075687    0.12241453
  912   14     0.45513    -3.29857     4.64716     -0.00147339    1.72027151   -
0.00085649    0.11980727
  913   14    -0.20172    -2.48736     5.01456     -0.00023278    0.86074563   -
0.00027044    0.11454120
  914   24     7.43841     0.46308    -0.05073     -0.00222779    0.95593850   -
0.00233047    0.17712324
  915   24     7.76470     0.30092    -1.23728     -0.00545891    1.91149563   -
0.00285583    0.17961382
  916   24     7.68104     0.56465    -2.44729     -0.00177797    0.95593850   -
0.00185992    0.17557813
  917   17     6.52672    -0.65436    -0.64710     -0.00685148    1.91149563   -
0.00358435    0.19051223
  918   17     6.67797    -0.59104    -2.14111     -0.00729239    1.91149563   -
0.00381502    0.19072440
  919   25     5.37054     8.38509    -0.58090     -0.00194960    1.19424595   -
0.00163250    0.16096974
  920   25     5.04620     8.08028     0.43629     -0.00195308    1.19424595   -
0.00163541    0.16191122
  921   19     3.68649     8.56119    -0.45914     -0.00752484    2.38860431   -
0.00315031    0.17126633];
```

[$N_{4,1,1,1}$] Computation ID = 64)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.33
%   total number of segments         =    818
%   number of charge corr segments   =    314
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N            -2.80260523658351   -0.11759239925055    0.00000000000000   3.4582
0.0000     0.00     0.00000    5.9148
% C            -0.24991359680785    1.28871533737700    0.00000000000000   3.7795  -
0.0129    10.39    -0.00124    6.2361
% C             2.12750528121207   -0.33159196769464    0.00000000000000   3.7795  -
0.0134    19.85    -0.00068    6.2361
% C            -3.07126400549647   -1.74229526928673   -2.32881902758126   3.7795  -
0.0552    43.09    -0.00128    6.2361
% C            -4.87919189033218    1.84078281803356    0.00000000000000   3.7795  -
0.0576    45.42    -0.00127    6.2361
% C            -3.07126400549647   -1.74229526928673    2.32881902758126   3.7795  -
0.0533    42.68    -0.00125    6.2361
% C             4.49711748146743    1.36068777990673    0.00000000000000   3.7795
0.0064    25.62     0.00025    6.2361
% C             6.95280441449657   -0.16620991658045    0.00000000000000   3.7795
0.0432    58.63     0.00074    6.2361
% H            -0.30797492694238    2.51542910253383    1.67418200096325   2.4566  -
0.0592    22.94    -0.00258    4.9133
% H            -0.30797492694238    2.51542910253383   -1.67418200096325   2.4566  -
0.0593    22.80    -0.00260    4.9133
% H             2.18783320465962   -1.57114381271760   -1.67051511083903   2.4566  -
0.0338    20.45    -0.00165    4.9133
% H             2.18783320465962   -1.57114381271760    1.67051511083903   2.4566  -
0.0338    20.52    -0.00165    4.9133
% H            -4.94985485095331   -2.61216240574774   -2.31628680149671   2.4566  -
0.0632    22.78    -0.00278    4.9133
% H            -1.62068626564072   -3.21315525600401   -2.30809809083122   2.4566  -
0.0524    18.36    -0.00285    4.9133
% H            -2.85398752300922   -0.55036479982550   -4.00754627907134   2.4566  -
0.0653    24.08    -0.00271    4.9133
% H            -6.71299040830803    0.87888517971159    0.00000000000000   2.4566  -
0.0615    22.48    -0.00274    4.9133
% H            -4.69602514319878    3.01325213538323   -1.69581682954840   2.4566  -
0.0617    22.56    -0.00274    4.9133
% H            -4.69602514319878    3.01325213538323    1.69581682954840   2.4566  -
0.0617    22.49    -0.00274    4.9133
```

```
% H            -1.62068626564072   -3.21315525600401    2.30809809083122   2.4566  -
0.0521    18.72    -0.00279    4.9133
% H            -4.94985485095331   -2.61216240574774    2.31628680149671   2.4566  -
0.0634    22.86    -0.00278    4.9133
% H            -2.85398752300922   -0.55036479982550    4.00754627907134   2.4566  -
0.0655    24.22    -0.00270    4.9133
% H             4.44831115164782    2.61732385283268    1.66286040357910   2.4566  -
0.0273    24.94    -0.00110    4.9133
% H             4.44831115164782    2.61732385283268   -1.66286040357910   2.4566  -
0.0272    24.94    -0.00109    4.9133
% H             7.09730672640345   -1.38291705432802   -1.68152783587258   2.4566  -
0.0226    25.08    -0.00090    4.9133
% H             7.09730672640345   -1.38291705432802    1.68152783587258   2.4566  -
0.0225    24.94    -0.00090    4.9133
% H             8.59995721991541    1.09839018281650    0.00000000000000   2.4566  -
0.0246    24.15    -0.00102    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -332.242314
%   Total energy + OC corr.      =       -332.237648
%   Dielectric energy            =         -0.086675      -2.359      -54.39
%   Diel. energy + OC corr.      =         -0.082009      -2.232      -51.46
%
%   Surface area of cavity [au]
acosmo =           654.984;
%   Total Volume of cavity [au]
vcosmo =          1262.523;
%
%
% $screening_charge
%   cosmo           =   -1.03422
%   corrected total =   -1.00003
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    2    -0.86569     4.99473    -0.41304     -0.00020993    0.49769306   -
0.00042181    0.16052239
    2    2    -0.78369     5.01240     0.36558     -0.00032003    0.66359074   -
0.00048227    0.15957173
    3    2     0.99799     4.79256     0.67097     -0.00046107    0.49769306   -
0.00092640    0.15118334
    4    2     0.72155     4.93196    -0.25965     -0.00051561    0.82948843   -
0.00062161    0.15054686
    5    2    -0.03719     5.03514    -0.45099     -0.00031071    0.66359074   -
0.00046823    0.15528709
    6    2     0.09513     5.03342     0.37751     -0.00024788    0.66359074   -
0.00037355    0.15410013
    7    3     2.09932     0.40706     3.70647     -0.00012882    0.33179537   -
0.00038826    0.14900535
    8    3     1.95965    -4.10551    -0.11689      0.00015675    0.66359074
0.00023622    0.14504522
```

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    9    3     1.96754     0.31576    -3.72015     -0.00033429    0.33179537   -
0.00100751    0.15109853
   10    3     3.44341    -3.86337     0.28142      0.00046383    0.82948843
0.00055917    0.12796315
   11    3     2.56602    -4.08106     0.18308      0.00056777    0.99538612
0.00057040    0.13716052
   12    3     1.80249     0.14541     3.73513     -0.00025661    0.16589769   -
0.00154681    0.15388520
   13    3     3.15929    -3.92685    -0.54202      0.00028193    0.49769306
0.00056646    0.13188151
   14    3     2.35801     0.23506    -3.72960     -0.00003838    0.16589769   -
0.00023136    0.14648681
   15    4    -5.49870    -0.85026    -5.08493     -0.00049897    0.99538612   -
0.00050128    0.15791493
   16    4    -3.54741    -4.46220    -4.90948     -0.00123747    1.32718149   -
0.00093241    0.14826525
   17    4    -3.42616    -5.35419    -1.27401     -0.00009965    1.32718149   -
0.00007509    0.16092603
   18    4    -0.50011    -1.49966    -5.08826     -0.00021140    0.82948843   -
0.00025485    0.16045414
   19    4    -4.26834    -5.25216    -1.59923     -0.00037056    0.82948843   -
0.00044673    0.16062017
   20    4    -4.57137    -4.50873    -4.42189     -0.00190095    1.49307918   -
0.00127318    0.15267866
   21    4    -6.00434    -1.48150    -4.69808     -0.00038674    0.82948843   -
0.00046624    0.15773805
   22    4    -0.97841    -2.33032    -5.42050     -0.00067145    1.16128380   -
0.00057819    0.15452044
   23    4    -0.63964    -2.93956    -4.96284     -0.00050272    0.66359074   -
0.00075758    0.15584920
   24    4    -5.87192    -0.40759    -4.48733     -0.00012507    0.66359074   -
0.00018848    0.16128232
   25    4    -5.03240    -1.94039    -5.55358     -0.00112268    1.82487455   -
0.00061521    0.15277769
   26    4    -4.36980    -3.51398    -5.40442     -0.00138795    1.49307918   -
0.00092959    0.14895811
   27    4    -3.73075    -5.12535    -3.87945     -0.00075061    1.16128380   -
0.00064636    0.15041887
   28    4    -3.39447    -5.50674    -2.42301     -0.00055715    1.16128380   -
0.00047977    0.15532991
   29    4    -2.13589    -2.67604    -5.86966     -0.00151791    1.65897686   -
0.00091497    0.15236010
   30    4    -2.87689    -3.67992    -5.56799     -0.00198731    1.99077223   -
0.00099826    0.14829292
   31    4    -2.51413    -4.70619    -4.60683     -0.00160637    1.32718149   -
0.00121036    0.15202076
   32    4    -4.15313    -5.30468    -2.97949     -0.00054947    0.99538612   -
0.00055202    0.15409277
   33    4    -5.27548    -2.95802    -5.14801     -0.00140040    1.32718149   -
0.00105517    0.15312066
   34    4    -6.36295    -0.87841    -3.97285     -0.00026483    0.49769306   -
0.00053211    0.16471315
   35    4    -1.57170    -3.67427    -5.21033     -0.00154746    1.49307918   -
0.00103642    0.15223766
   36    4    -3.73357    -2.59074    -5.95178     -0.00182104    1.65897686   -
0.00109769    0.15142561
```

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   37    4    -2.95813    -5.32202    -3.53596     -0.00057102    0.82948843   -
0.00068840    0.15398070
   38    5    -7.16948     2.30810     2.96990     -0.00049678    0.99538612   -
0.00049909    0.15795296
   39    5    -7.82913     4.10802    -0.66460     -0.00126874    1.32718149   -
0.00095597    0.14868006
   40    5    -6.88117     1.58697    -3.19562     -0.00009869    1.16128380   -
0.00008498    0.16150370
   41    5    -3.60965     5.33913     0.65885     -0.00035580    0.82948843   -
0.00042894    0.16197092
   42    5    -7.48837     1.29222    -2.67873     -0.00041933    0.82948843   -
0.00050552    0.16150382
   43    5    -8.38789     3.12452    -0.57029     -0.00195216    1.49307918   -
0.00130747    0.15311178
   44    5    -7.74293     1.83752     2.46639     -0.00040531    0.82948843   -
0.00048862    0.15783282
   45    5    -4.86340     5.60747     0.30985     -0.00082762    1.65897686   -
0.00049888    0.15450247
   46    5    -4.55548     5.56125    -0.58104     -0.00051648    0.82948843   -
0.00062265    0.15695570
   47    5    -6.87117     1.49073     3.19274     -0.00012274    0.82948843   -
0.00014797    0.16195496
   48    5    -7.66224     3.17849     2.17929     -0.00101639    1.82487455   -
0.00055697    0.15292646
   49    5    -8.05354     3.79351     0.62812     -0.00139773    1.49307918   -
0.00093614    0.14925469
   50    5    -7.93795     3.34404    -1.63353     -0.00076284    1.16128380   -
0.00065689    0.15104343
   51    5    -7.34516     2.50677    -2.78563     -0.00060115    1.16128380   -
0.00051766    0.15627680
   52    5    -6.16680     5.32454     0.69976     -0.00168357    1.65897686   -
0.00101483    0.15235804
   53    5    -7.15842     4.85544     0.03304     -0.00197180    1.99077223   -
0.00099047    0.14850237
   54    5    -7.12013     4.55022    -1.38612     -0.00159549    1.32718149   -
0.00120217    0.15239926
   55    5    -3.52732     5.35722    -0.30231     -0.00051152    1.32718149   -
0.00038542    0.16036082
   56    5    -7.98489     2.43439    -2.07039     -0.00060386    0.99538612   -
0.00060666    0.15483200
   57    5    -8.26817     2.93299     1.26729     -0.00144004    1.32718149   -
0.00108503    0.15335677
   58    5    -7.35678     0.93685     2.70713     -0.00035233    0.49769306   -
0.00070792    0.16482458
   59    5    -6.08922     5.36721    -0.61995     -0.00144636    1.49307918   -
0.00096871    0.15213908
   60    5    -7.28066     4.40521     1.39313     -0.00193816    1.65897686   -
0.00116829    0.15165024
   61    5    -7.36967     3.58753    -2.24292     -0.00065703    0.82948843   -
0.00079209    0.15472484
   62    6    -0.52491    -1.75002     5.12173     -0.00040378    0.82948843   -
0.00048679    0.15843524
   63    6    -3.56791    -4.45846     4.90951     -0.00126777    1.32718149   -
0.00095523    0.14828253
   64    6    -4.01194    -5.24795     1.27542     -0.00010595    1.32718149   -
0.00007983    0.16125691
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   65    6    -5.51553    -0.22256     4.77834     -0.00039160    0.99538612   -
0.00039341    0.16285106
   66    6    -3.18600    -5.44833     1.59652     -0.00035637    0.82948843   -
0.00042963    0.16003795
   67    6    -2.62779    -4.86106     4.41707     -0.00187853    1.49307918   -
0.00125816    0.15236900
   68    6    -0.69180    -2.83259     5.05530     -0.00068848    0.99538612   -
0.00069168    0.15507814
   69    6    -5.27882    -1.48535     5.38576     -0.00079112    1.65897686   -
0.00047687    0.15462490
   70    6    -5.94393    -1.77994     4.78453     -0.00052514    0.82948843   -
0.00063309    0.15716694
   71    6    -1.46530    -2.56173     5.65052     -0.00085231    1.32718149   -
0.00064219    0.15301817
   72    6    -2.46264    -3.85972     5.39969     -0.00138327    1.49307918   -
0.00092645    0.14893440
   73    6    -3.83383    -5.04726     3.99610     -0.00099554    1.32718149   -
0.00075011    0.15028890
   74    6    -3.93768    -5.42086     2.36846     -0.00043431    1.16128380   -
0.00037399    0.15510883
   75    6    -4.25796    -2.29130     5.87488     -0.00162719    1.65897686   -
0.00098084    0.15228046
   76    6    -3.91798    -3.49116     5.57053     -0.00196634    1.99077223   -
0.00098773    0.14830610
   77    6    -4.67970    -4.25400     4.65011     -0.00137958    1.16128380   -
0.00118797    0.15250609
   78    6    -6.11395    -0.79590     4.36121     -0.00031243    1.32718149   -
0.00023540    0.16074648
   79    6    -3.32226    -5.42151     3.15616     -0.00055513    0.99538612   -
0.00055770    0.15312645
   80    6    -1.52165    -3.71611     5.15495     -0.00127277    1.16128380   -
0.00109600    0.15272846
   81    6    -5.13982    -3.02736     5.21912     -0.00147574    1.49307918   -
0.00098839    0.15217335
   82    6    -2.73165    -2.77237     5.94929     -0.00180366    1.65897686   -
0.00108721    0.15145860
   83    6    -4.34668    -5.18437     3.22856     -0.00043799    0.66359074   -
0.00066003    0.15472985
   84    7     6.76380     4.38344     0.09723      0.00088008    0.99538612
0.00088416    0.09380010
   85    7     3.35162     4.94499    -0.35348      0.00106662    1.16128380
0.00091848    0.11974701
   86    7     4.53483     0.59067    -3.69997      0.00022844    0.33179537
0.00068848    0.11949302
   87    7     4.99909     1.01149    -3.72964      0.00004744    0.16589769
0.00028596    0.11554615
   88    7     3.67465     5.02525     0.42299      0.00089033    0.82948843
0.00107335    0.11584909
   89    7     6.36880     4.48374     1.01376      0.00054872    0.99538612
0.00055127    0.09804122
   90    7     4.16520     0.77743     3.71941      0.00013851    0.66359074
0.00020873    0.12432064
   91    7     5.89457     4.86394    -0.24222      0.00125817    1.32718149
0.00094800    0.09755815
   92    7     4.49183     5.13291    -0.23375      0.00116396    0.99538612
0.00116935    0.10703485
```

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   93    7     6.48177     4.43185    -0.95574      0.00056668    0.82948843
0.00068317    0.09692306
   94    7     4.21629     0.82513    -3.73074      0.00004396    0.16589769
0.00026497    0.12368766
   95    7     5.23370     5.05700     0.28124      0.00104977    0.99538612
0.00105463    0.10154110
   96    7     4.77501     0.84834     3.73425      0.00010286    0.16589769
0.00062000    0.11750616
   97    8     9.61174     0.52062    -2.59662      0.00116572    0.82948843
0.00140535    0.07544704
   98    8     9.87490    -2.56255     0.05580      0.00123744    1.32718149
0.00093238    0.07122902
   99    8     6.13265    -3.81331     0.55711      0.00137487    1.16128380
0.00118392    0.09779025
  100    8     8.18564     1.97707     2.85844      0.00174666    1.65897686
0.00105285    0.08486699
  101    8     9.08639     1.27533     2.76659      0.00076478    0.66359074
0.00115249    0.07920102
  102    8     7.43178     1.10350     3.52742      0.00104756    0.99538612
0.00105242    0.08922130
  103    8     8.00987     0.71843     3.51913      0.00077350    0.66359074
0.00116562    0.08470037
  104    8     6.78851    -3.93205    -0.27522      0.00141181    0.99538612
0.00141835    0.09079811
  105    8     9.42123    -2.87007    -0.93819      0.00124499    1.49307918
0.00083384    0.07563422
  106    8     9.14189     0.01020    -3.07586      0.00165989    1.32718149
0.00125069    0.07777604
  107    8     6.82161     0.49138    -3.71948      0.00069567    0.82948843
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  741   22     2.75788     4.66078     1.97127     -0.00038200    0.86769087   -
0.00044025    0.13335246
  742   22     2.77187     4.12077     2.98653     -0.00186617    1.73472855   -
0.00107577    0.13751901
  743   22     2.79968     2.89852     3.66931     -0.00179064    1.73472855   -
0.00103223    0.14019940
  744    9     1.29958     4.45039     2.37731     -0.00300597    1.73472855   -
0.00173282    0.15455121
  745    9     1.32163     3.53911     3.44030     -0.00338148    1.73472855   -
0.00194929    0.15751021
  746    9     1.34603     2.43720     3.76855     -0.00118521    0.86769087   -
0.00136594    0.15869769
  747   10    -2.00326     2.81911    -3.75494     -0.00385573    0.91558646   -
0.00421121    0.18852935
  748   15    -2.55498     2.14831    -4.25291     -0.00376282    0.91558646   -
0.00410973    0.18874534
  749   17    -2.95281     2.92658    -3.75910     -0.00377060    0.91558646   -
0.00411824    0.18922610
  750   15    -2.07492     1.84593    -4.83794     -0.00211281    0.93141853   -
0.00226838    0.17989714
  751   15    -1.07829     1.08522    -4.92590     -0.00493398    1.86325710   -
0.00264804    0.17727880
  752   10    -0.90173     2.51046    -4.18795     -0.00518883    1.86325710   -
0.00278482    0.17929463
  753   10     0.05916     1.70045    -4.17214     -0.00167256    0.93141853   -
0.00179572    0.17199842
  754   17    -2.93007     4.96514    -1.95104     -0.00121085    0.76754919   -
0.00157755    0.17109812
  755   17    -2.97776     4.50179    -2.94138     -0.00393594    1.53498578   -
0.00256415    0.17671015
  756   17    -3.06662     3.68709    -3.66673     -0.00193196    0.76754919   -
0.00251706    0.18060465
  757   10    -1.60456     4.66103    -2.33365     -0.00353165    1.53498578   -
0.00230077    0.17344763
  758   10    -1.68976     3.86359    -3.40415     -0.00427110    1.53498578   -
0.00278250    0.17925826
  759   23     2.80914     2.46852    -3.76507     -0.00054177    0.86770820   -
0.00062437    0.13935275
  760   23     2.78476     3.57045    -3.43682     -0.00187579    1.73476340   -
0.00108129    0.13890337
  761   23     2.76270     4.48174    -2.37380     -0.00169953    1.73476340   -
0.00097969    0.13595067
  762   10     1.33662     2.86716    -3.67280     -0.00316773    1.73476340   -
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0.00194486    0.15586472
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0.00131363    0.15191210
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  765   14     0.40394    -3.54491    -3.94390     -0.00142930    0.77529512   -
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  766   14     0.57857    -4.28682    -3.07630     -0.00440993    1.55125014   -
0.00284282    0.16668696
  767   14     0.55106    -4.64872    -1.97998     -0.00176064    0.77529512   -
0.00227092    0.16713760
  768   11     1.64221    -3.34836    -3.43780     -0.00344966    1.55125014   -
0.00222379    0.15830164
  769   11     1.73396    -4.03674    -2.21301     -0.00310560    1.55125014   -
0.00200200    0.15693863
  770   15    -0.24152    -0.34832    -4.88278     -0.00012220    0.34242510   -
0.00035687    0.16450614
  771   11     1.34899    -0.71652    -4.16003      0.00016258    0.34242510
0.00047478    0.15484764
  772   24     5.47805    -3.49441    -2.03889      0.00011677    0.85344027
0.00013682    0.11134711
  773   24     5.45537    -2.95923    -3.00310     -0.00096510    1.70572570   -
0.00056580    0.11564654
  774   24     5.40890    -1.78553    -3.66003     -0.00104491    1.70572570   -
0.00061259    0.11662130
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0.00090452    0.13093363
  776   11     3.91840    -2.48704    -3.42935     -0.00171304    1.70572570   -
0.00100429    0.13283635
  777   11     3.87728    -1.43324    -3.75255     -0.00042223    0.85344027   -
0.00049474    0.13155207
  778   19     0.55106    -4.64872     1.97997     -0.00188990    0.77527789   -
0.00243771    0.16713657
  779   19     0.57856    -4.28684     3.07627     -0.00448873    1.55121563   -
0.00289369    0.16668258
  780   19     0.40393    -3.54496     3.94387     -0.00145221    0.77527789   -
0.00187314    0.16298800
  781   12     1.73395    -4.03675     2.21301     -0.00308105    1.55121563   -
0.00198622    0.15691969
  782   12     1.64219    -3.34839     3.43779     -0.00343194    1.55121563   -
0.00221242    0.15826531
  783   21    -0.24362    -0.39403     4.89825      0.00001647    0.34229729
0.00004812    0.16410538
  784   12     1.35107    -0.67072     4.14457      0.00015100    0.34229729
0.00044112    0.15492397
  785   25     5.39298    -1.37517     3.75594     -0.00013089    0.85341667   -
0.00015337    0.11514475
  786   25     5.43410    -2.42893     3.43274     -0.00109525    1.70567836   -
0.00064212    0.11651890
  787   25     5.47035    -3.31524     2.42065     -0.00075892    1.70567836   -
0.00044494    0.11391877
  788   12     3.89324    -1.84365     3.65662     -0.00159243    1.70567836   -
0.00093361    0.13288994
  789   12     3.93970    -3.01732     2.99971     -0.00174885    1.70567836   -
0.00102531    0.13216417
  790   12     3.96238    -3.55250     2.03554     -0.00040737    0.85341667   -
0.00047734    0.12855606
  791   13    -6.96799    -2.50379    -0.50234     -0.00400035    0.92643156   -
0.00431802    0.19047145
  792   16    -7.35359    -1.74939     0.00001     -0.00395527    0.92643156   -
0.00426936    0.19066210
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  793   20    -6.96798    -2.50379     0.50237     -0.00384966    0.92643156   -
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  794   16    -7.75679    -0.27089    -2.15557     -0.00130726    0.75967897   -
0.00172080    0.17242904
  795   16    -8.01208    -0.92459    -1.36463     -0.00381995    1.51889324   -
0.00251495    0.17761403
  796   16    -7.88560    -1.45990    -0.46155     -0.00172202    0.75967897   -
0.00226677    0.18152573
  797   13    -7.33683    -1.59331    -2.57480     -0.00360730    1.51889324   -
0.00237495    0.17545536
  798   13    -7.41723    -2.33542    -1.51749     -0.00418473    1.51889324   -
0.00275512    0.18099670
  799   20    -6.94347    -3.30160     0.71066     -0.00215315    0.98253110   -
0.00219143    0.18113508
  800   20    -6.06924    -4.28337     0.71065     -0.00524843    1.96606782   -
0.00266950    0.17785661
  801   13    -6.63736    -3.70684    -0.71063     -0.00570299    1.96606782   -
0.00290071    0.18156458
  802   13    -5.66855    -4.59542    -0.71064     -0.00178113    0.98253110   -
0.00181279    0.17297311
  803   19    -1.61373    -5.31681     0.70789     -0.00212132    1.07113905   -
0.00198044    0.17097780
  804   19    -0.55104    -5.02457     0.70789     -0.00225652    1.07113905   -
0.00210665    0.17306712
  805   14    -1.09384    -5.12904    -0.70792     -0.00617438    2.14518871   -
0.00287825    0.17595551
  806   17    -3.65978     3.04710    -4.13631     -0.00208231    0.97002699   -
0.00214665    0.18036794
  807   17    -4.83292     2.49165    -4.21486     -0.00513574    1.94089341   -
0.00264607    0.17747654
  808   15    -3.55273     1.75903    -4.91027     -0.00551223    1.94089341   -
0.00284005    0.18061408
  809   15    -4.69845     1.14490    -4.87651     -0.00180313    0.97002699   -
0.00185884    0.17264749
  810   20    -7.21674    -1.34011     2.86504     -0.00131057    0.75968342   -
0.00172515    0.17251156
  811   20    -7.47204    -1.99383     2.07410     -0.00384395    1.51890216   -
0.00253074    0.17766861
  812   20    -7.34558    -2.52914     1.17102     -0.00185901    0.75968342   -
0.00244708    0.18146955
  813   16    -7.87680    -0.52404     1.86541     -0.00358855    1.51890216   -
0.00236260    0.17537405
  814   16    -7.95722    -1.26617     0.80809     -0.00420803    1.51890216   -
0.00277044    0.18105200
  815   21    -3.09464     1.95384     4.84554     -0.00220497    0.97003955   -
0.00227307    0.18003316
  816   21    -4.26780     1.39837     4.92408     -0.00507704    1.94091899   -
0.00261579    0.17722834
  817   18    -4.11786     2.85230     4.20106     -0.00551237    1.94091899   -
0.00284008    0.18088062
  818   18    -5.26359     2.23816     4.16730     -0.00184168    0.97003955   -
0.00189856    0.17284557];
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[OMIM] Computation ID = 65)

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% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.44
%   total number of segments         =   1342
%   number of charge corr segments   =    489
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N             2.85966218536386    4.43796587059494   -3.94263914888906   3.4582  -
0.0038     3.71    -0.00102    5.9148
% N             6.21094496702215    6.87056741829561   -3.93938262354211   3.4582  -
0.0081     6.24    -0.00129    5.9148
% C            -1.03242667251860   -1.02038025249929   -1.03512667178524   3.7795
0.0073    19.97     0.00037    6.2361
% C            -1.71729676632348   -1.84835056954606    1.65948372884844   3.7795
0.0144    20.36     0.00070    6.2361
% C             0.62062169227693    1.36397721083991   -1.09872199545597   3.7795  -
0.0075    22.99    -0.00033    6.2361
% C            -3.35024509320559   -4.24324360374170    1.73217114095723   3.7795
0.0173    20.35     0.00085    6.2361
% C             1.24547919795090    2.14699507242466   -3.81414769156193   3.7795  -
0.0297    21.82    -0.00136    6.2361
% C            -4.07586431520403   -5.06602491237322    4.41481397785091   3.7795
0.0180    20.04     0.00090    6.2361
% C            -5.69787288148827   -7.46833261772235    4.49080302495899   3.7795
0.0226    26.19     0.00086    6.2361
% C             5.40211820490037    4.45617505988606   -3.96856878780767   3.7795  -
0.0764    46.59    -0.00164    6.2361
% C             2.02155894707528    6.91855156137995   -3.88884839520758   3.7795  -
0.0338    48.55    -0.00070    6.2361
% C            -6.43321771504927   -8.26657549624957    7.17392804437073   3.7795
0.0584    58.60     0.00100    6.2361
% C             4.11506632492549    8.44124524424253   -3.89410535628455   3.7795  -
0.0416    53.03    -0.00078    6.2361
% C             8.86439337398821    7.69336999579466   -4.06186389574583   3.7795  -
0.0807    63.34    -0.00127    6.2361
% H            -2.78129460959569   -0.68274500979885   -2.12114796724349   2.4566  -
0.0225    25.32    -0.00089    4.9133
% H            -0.04162269929505   -2.57778937779793   -2.00736086384769   2.4566  -
0.0223    25.50    -0.00087    4.9133
% H            -2.72067599763486   -0.29391652890313    2.62396769864829   2.4566  -
0.0153    25.36    -0.00060    4.9133
% H             0.03337406396315   -2.16736496123686    2.74936406804161   2.4566  -
0.0156    25.42    -0.00061    4.9133
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% H             2.39573334831349    1.03012723129729   -0.05898537269361   2.4566  -
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% H            -0.35053020261114    2.93261124884977   -0.13106336702435   2.4566  -
0.0323    23.99    -0.00135    4.9133
% H            -2.33412945174192   -5.79925870642382    0.78223919804522   2.4566  -
0.0126    25.35    -0.00050    4.9133
% H            -5.08366671885206   -3.92742394524329    0.61335823874447   2.4566  -
0.0127    25.28    -0.00050    4.9133
% H             2.25296444886337    0.64137363457872   -4.82649454261041   2.4566  -
0.0606    24.44    -0.00248    4.9133
% H            -0.46899248844017    2.57579134023250   -4.90124473629355   2.4566  -
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0.0111    25.75    -0.00043    4.9133
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0.0141    24.91    -0.00057    4.9133
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% H            -7.57906039803882  -10.00218520365083    7.16059157058469   2.4566  -
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% H            -7.54672362946534   -6.78695573557185    8.12675468676853   2.4566  -
0.0167    25.10    -0.00067    4.9133
% H            -4.75086603619651   -8.63497707708348    8.34454337201023   2.4566  -
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0.0832    24.59    -0.00338    4.9133
% H             9.31313087846428    8.32672581906096   -5.98597871063120   2.4566  -
0.0623    25.16    -0.00248    4.9133
% H            10.08726943666237    6.10587977162191   -3.54106060645951   2.4566  -
0.0636    23.26    -0.00273    4.9133
% H             9.15317586288067    9.24346987209115   -2.71730613233732   2.4566  -
0.0631    24.52    -0.00258    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -580.624282
%   Total energy + OC corr.      =       -580.619784
%   Dielectric energy            =         -0.084022      -2.286      -52.73
%   Diel. energy + OC corr.      =         -0.079525      -2.164      -49.90
%
%   Surface area of cavity [au]
acosmo =          1007.974;
%   Total Volume of cavity [au]
vcosmo =          1944.448;
%
%
% $screening_charge
%   cosmo           =   -1.04674
%   corrected total =   -1.00075
%
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%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1     2.55488     4.25095    -7.38230      0.00003604    0.69446845
0.00005190    0.15056114
    2    1     2.79094     4.71721    -7.38886     -0.00004264    0.13889369   -
0.00030697    0.14948517
    3    2     6.51252     7.00150    -0.49683      0.00003620    0.55557476
0.00006516    0.15342476
    4    2     6.00910     6.98186    -7.38988     -0.00014714    0.13889369   -
0.00105940    0.15726514
    5    2     6.37207     6.82517    -7.39351     -0.00012381    0.13889369   -
0.00089142    0.15910925
    6    2     6.05005     6.91597    -0.48521     -0.00007425    0.13889369   -
0.00053460    0.15223989
    7    3    -2.32915    -3.64699    -3.42337      0.00134491    1.16128380
0.00115812    0.08856096
    8    3     2.24437    -2.74881    -0.28726      0.00014765    0.33179537
0.00044499    0.11096498
    9    3     2.37837    -2.64204    -0.89071      0.00002304    0.16589769
0.00013888    0.11694819
   10    3    -2.94375    -3.04200    -3.59328      0.00124639    0.99538612
0.00125217    0.09025117
   11    3    -4.08519     1.13910    -0.48591      0.00023974    0.66359074
0.00036128    0.10479076
   12    3    -1.31460    -2.17965    -4.62130      0.00093391    0.82948843
0.00112588    0.10731389
   13    3    -1.92773    -2.82244    -4.23438      0.00157747    1.16128380
0.00135838    0.09692074
   14    3     2.04542    -3.09114    -0.31196      0.00006974    0.16589769
0.00042041    0.10848464
   15    3    -2.14626    -1.92880    -4.53060      0.00058635    0.49769306
0.00117814    0.10434657
   16    3    -3.81615     1.53099    -0.87472      0.00007772    0.16589769
0.00046847    0.11044579
   17    4     0.12922     0.40971     4.06274      0.00159141    1.16128380
0.00137039    0.08623326
   18    4     1.10985    -4.30999     1.17799      0.00026198    0.33179537
0.00078959    0.08966985
   19    4     1.02379    -4.44744     1.78396      0.00006112    0.16589769
0.00036843    0.08765688
   20    4    -0.66442     0.77140     4.17194      0.00148512    0.99538612
0.00149201    0.08483916
   21    4    -4.79164     0.19332     0.84445      0.00036590    0.66359074
0.00055139    0.09058968
   22    4    -0.94345    -1.01339     5.26339      0.00132875    0.82948843
0.00160189    0.07164023
   23    4    -0.54186    -0.22690     4.86469      0.00187417    1.16128380
0.00161388    0.07686226
   24    4     1.35621    -4.00009     1.20355      0.00009044    0.16589769
0.00054518    0.09294053
   25    4    -1.46989    -0.33292     5.11294      0.00075984    0.49769306
0.00152673    0.07383684
   26    4    -5.08275    -0.18200     1.23369      0.00015062    0.16589769
0.00090792    0.08621358
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   27    5     1.04975     2.69125     2.41387      0.00095590    1.16128380
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0.00094469    0.14243244
 1300   20    -1.57166     5.39304    -0.40917     -0.00050381    0.84182653   -
0.00059847    0.13950955
 1301   27    -4.23056    -9.08777     0.91726      0.00035365    0.87647144
0.00040350    0.05811290
 1302   27    -3.23890    -9.39605     1.39211     -0.00041228    1.75201686   -
0.00023532    0.06350536
 1303   27    -2.31545    -9.18684     2.41057     -0.00040752    1.75201686   -
0.00023260    0.06460576
 1304   21    -3.12907    -8.23303     0.22105     -0.00022203    1.75201686   -
0.00012673    0.06676801
 1305   21    -1.98738    -8.38820     0.99968     -0.00049706    1.75201686   -
0.00028371    0.07047486
 1306   21    -1.38990    -8.03833     1.90771      0.00018320    0.87647144
0.00020902    0.06897328
 1307   28    -8.32519    -4.85226     2.35891      0.00019013    0.87676431
0.00021686    0.06223489
 1308   28    -8.34088    -5.58433     1.48091     -0.00050601    1.75262041   -
0.00028872    0.06407818
 1309   28    -7.69607    -6.61900     0.80867     -0.00022255    1.75262041   -
0.00012698    0.06076252
 1310   22    -7.63724    -4.12174     1.16867     -0.00038178    1.75262041   -
0.00021783    0.06952772
 1311   22    -7.38986    -5.10667     0.21633     -0.00048879    1.75262041   -
0.00027889    0.06852168
 1312   22    -6.68767    -5.92859    -0.15573      0.00034575    0.87676431
0.00039435    0.06331110
 1313   29     5.88982     0.23007    -3.67378     -0.00225227    0.79525893   -
0.00283213    0.18502499
 1314   29     6.04113     0.30699    -4.69082     -0.00535659    1.58931100   -
0.00337038    0.18628999
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 1315   29     6.00429     0.73379    -5.62874     -0.00199892    0.79525893   -
0.00251355    0.18304281
 1316   23     4.61393    -0.42932    -4.31112     -0.00343686    1.58931100   -
0.00216249    0.17270270
 1317   23     4.68541    -0.11478    -5.53188     -0.00378314    1.58931100   -
0.00238037    0.17324786
 1318   30    -1.73679     6.16140    -5.45004     -0.00188421    0.99926693   -
0.00188559    0.16358278
 1319   30    -2.10207     5.93944    -4.26092     -0.00635295    1.99783359   -
0.00317992    0.16910688
 1320   24    -2.06696     4.59403    -5.32791     -0.00495107    1.99783359   -
0.00247822    0.16197278
 1321   24    -2.31240     4.35384    -4.11185     -0.00162295    0.99926693   -
0.00162414    0.15893191
 1322   32    -6.45109    -4.43756     8.83340      0.00038216    0.85024654
0.00044947    0.05093344
 1323   32    -7.38520    -4.16495     8.33069     -0.00033834    1.69927768   -
0.00019911    0.05601075
 1324   32    -8.24154    -4.37484     7.32581     -0.00043760    1.69927768   -
0.00025752    0.05656800
 1325   25    -6.05685    -3.30235     7.80640     -0.00008655    1.69927768   -
0.00005093    0.05788340
 1326   25    -7.12541    -3.17484     7.01326     -0.00037081    1.69927768   -
0.00021821    0.06098982
 1327   25    -7.67663    -3.51100     6.12853      0.00022858    0.85024654
0.00026884    0.05912984
 1328   33    -2.21787    -8.69459     7.45245      0.00013853    0.86043104
0.00016100    0.05536855
 1329   33    -2.20124    -7.97977     8.29843     -0.00049523    1.71966369   -
0.00028798    0.05755224
 1330   33    -2.80754    -6.96725     8.95622     -0.00015140    1.71966369   -
0.00008804    0.05419135
 1331   26    -1.44250    -7.42442     6.91735     -0.00025376    1.71966369   -
0.00014756    0.06133162
 1332   26    -1.67292    -6.46300     7.83825     -0.00033680    1.71966369   -
0.00019585    0.06056835
 1333   26    -2.33463    -5.65596     8.20940      0.00035011    0.86043104
0.00040690    0.05540525
 1334   36     9.93075     3.67749    -2.43965     -0.00222275    0.95120288   -
0.00233677    0.17691423
 1335   36    10.25216     3.50863    -3.62043     -0.00544759    1.90197867   -
0.00286417    0.17936485
 1336   36    10.17225     3.76575    -4.82606     -0.00179439    0.95120288   -
0.00188644    0.17534811
 1337   29     9.00497     2.56806    -3.02891     -0.00691336    1.90197867   -
0.00363483    0.19022206
 1338   29     9.15553     2.62308    -4.51667     -0.00721662    1.90197867   -
0.00379427    0.19042539
 1339   37     7.98678    11.65089    -3.14157     -0.00104009    0.80339621   -
0.00129461    0.15988954
 1340   37     7.70364    11.42119    -2.20677     -0.00318937    1.60515639   -
0.00198695    0.16244016
 1341   34     6.37185    11.97163    -3.14266     -0.00442889    1.60515639   -
0.00275917    0.16814711
 1342   34     6.07631    11.67025    -2.23239     -0.00138544    0.80339621   -
0.00172448    0.16451168];
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[HMIM] Computation ID = 66)

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% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.44
%   total number of segments         =   1133
%   number of charge corr segments   =    428
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N             1.64874690600010    2.78302946324741   -2.71334037015991   3.4582  -
0.0038     3.70    -0.00103    5.9148
% N             4.96046197466420    5.26874437718224   -2.70941835319160   3.4582  -
0.0081     6.24    -0.00129    5.9148
% C            -0.62532761089140   -0.27557111320811    0.11931675756083   3.7795  -
0.0075    23.24    -0.00032    6.2361
% C            -2.25928802406345   -2.67388028468840    0.17463568740618   3.7795
0.0072    19.98     0.00036    6.2361
% C             0.06791098576965    0.46904071428218   -2.58998812507490   3.7795  -
0.0297    21.85    -0.00136    6.2361
% C            -2.99367250447691   -3.47690842030591    2.86302407406646   3.7795
0.0134    19.71     0.00068    6.2361
% C            -4.62649988132811   -5.87274419540161    2.93427584612028   3.7795
0.0203    26.52     0.00077    6.2361
% C             4.19048917219974    2.84179862670587   -2.73969810007597   3.7795  -
0.0764    46.99    -0.00163    6.2361
% C             0.77110318756051    5.25024803077836   -2.65888357683649   3.7795  -
0.0336    48.32    -0.00070    6.2361
% C            -5.36428884508520   -6.66284053641358    5.61893142464052   3.7795
0.0562    58.57     0.00096    6.2361
% C             2.83957318146902    6.80566473845491   -2.66370895281241   3.7795  -
0.0417    52.85    -0.00079    6.2361
% C             7.60016396010729    6.13471756659307   -2.83203538709959   3.7795  -
0.0808    63.35    -0.00127    6.2361
% H             1.12209635243850   -0.57546965335892    1.21450731598236   2.4566  -
0.0328    24.08    -0.00136    4.9133
% H            -1.64034896486842    1.29688141690376    1.03433215716201   2.4566  -
0.0323    23.62    -0.00137    4.9133
% H            -1.23507749507897   -4.23325495759334   -0.75917789132475   2.4566  -
0.0226    25.49    -0.00089    4.9133
% H            -3.98641683147807   -2.36070552466905   -0.95260774414335   2.4566  -
0.0226    25.33    -0.00089    4.9133
% H             1.13059428074725   -1.03760193912061   -3.54268194240284   2.4566  -
0.0605    24.38    -0.00248    4.9133
% H            -1.61994881576964    0.84824300399650   -3.73588904375445   2.4566  -
0.0596    24.83    -0.00240    4.9133
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% H            -4.01593856008083   -1.91570415614072    3.79686992176070   2.4566  -
0.0154    25.74    -0.00060    4.9133
% H            -1.26414535681993   -3.78624185844194    3.98923389534548   2.4566  -
0.0155    25.68    -0.00061    4.9133
% H            -3.59951006410146   -7.43174682280652    2.00457153920911   2.4566  -
0.0160    24.91    -0.00064    4.9133
% H            -6.34857828606957   -5.56277221124904    1.79962917437060   2.4566  -
0.0159    25.21    -0.00063    4.9133
% H             5.42183334897358    1.20461092225002   -2.78558699420141   2.4566  -
0.1091    27.55    -0.00396    4.9133
% H            -1.23075743186887    5.68941497572042   -2.61947526413067   2.4566  -
0.0855    25.93    -0.00330    4.9133
% H             2.97946350079719    8.85150098745613   -2.65478197352534   2.4566  -
0.0832    24.60    -0.00338    4.9133
% H            -6.50853514791559   -8.39839167175359    5.60332417090502   2.4566  -
0.0208    24.36    -0.00085    4.9133
% H            -6.48141735503425   -5.18325146866759    6.56641716243715   2.4566  -
0.0176    25.09    -0.00070    4.9133
% H            -3.68417606839191   -7.03009356249571    6.79226179928257   2.4566  -
0.0177    24.97    -0.00071    4.9133
% H             8.04244705209111    6.76359802895632   -4.75910475287659   2.4566  -
0.0623    25.15    -0.00247    4.9133
% H             8.84895666227404    4.57196468131708   -2.29822741836081   2.4566  -
0.0636    23.25    -0.00273    4.9133
% H             7.86008667823051    7.69772084247034   -1.49672503627826   2.4566  -
0.0631    24.31    -0.00259    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -501.984837
%   Total energy + OC corr.      =       -501.980373
%   Dielectric energy            =         -0.083780      -2.280      -52.57
%   Diel. energy + OC corr.      =         -0.079315      -2.158      -49.77
%
%   Surface area of cavity [au]
acosmo =           865.816;
%   Total Volume of cavity [au]
vcosmo =          1649.452;
%
%
% $screening_charge
%   cosmo           =   -1.04163
%   corrected total =   -1.00059
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1     1.34642     2.59188    -6.15299      0.00002574    0.69446845
0.00003707    0.15079620
    2    1     1.57502     3.06184    -6.15950     -0.00003958    0.13889369   -
0.00028499    0.14965439
    3    2     5.25957     5.40309     0.73322      0.00005353    0.55557476
0.00009634    0.15341115
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    4    2     4.75720     5.37820    -6.15989     -0.00014682    0.13889369   -
0.00105705    0.15736935
    5    2     5.12262     5.22735    -6.16355     -0.00012021    0.13889369   -
0.00086549    0.15919794
    6    2     4.79853     5.31015     0.74476     -0.00007591    0.13889369   -
0.00054653    0.15228533
    7    3    -0.31127     1.10781     3.62245      0.00094322    1.16128380
0.00081222    0.11100391
    8    3    -3.90307     1.42538    -0.68535     -0.00021222    0.33179537   -
0.00063960    0.13420021
    9    3     0.50017     0.77380     3.57132      0.00068313    0.99538612
0.00068629    0.11386650
   10    3     2.09970    -2.89338     0.04521     -0.00013059    0.66359074   -
0.00019679    0.13546031
   11    3     0.81596     2.38308     2.38614      0.00034026    0.66359074
0.00051276    0.12683482
   12    3     0.44689     1.87164     3.03892      0.00104755    1.16128380
0.00090206    0.11897199
   13    3    -4.00284     1.36636    -0.30594      0.00005677    0.16589769
0.00034220    0.13093572
   14    3     1.30046     1.84309     2.58647      0.00028080    0.49769306
0.00056420    0.12680009
   15    3     2.41989    -2.47896    -0.27550     -0.00015408    0.16589769   -
0.00092875    0.14408033
   16    4    -3.06738    -3.61601    -3.39521      0.00129245    1.16128380
0.00111295    0.10589725
   17    4    -5.10468    -0.22129     0.59032      0.00015282    0.33179537
0.00046058    0.10779324
   18    4    -5.47662    -0.72286     0.53039      0.00010212    0.16589769
0.00061555    0.10421888
   19    4    -2.46937    -4.24506    -3.25635      0.00116430    0.99538612
0.00116970    0.10454825
   20    4     1.14511    -4.24040     0.66484      0.00020543    0.66359074
0.00030957    0.11498807
   21    4    -4.07605    -5.04217    -2.14378      0.00109768    0.82948843
0.00132332    0.08773026
   22    4    -3.56045    -4.57759    -2.81990      0.00158439    1.16128380
0.00136434    0.09395141
   23    4    -5.04715    -0.12226     0.21049      0.00006243    0.16589769
0.00037635    0.11127757
   24    4    -3.27141    -5.34184    -2.30367      0.00060463    0.49769306
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   25    4     0.84416    -4.67726     0.97421      0.00009162    0.16589769
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   26    5    -0.43210    -0.02613    -6.30337     -0.00050561    1.16128380   -
0.00043539    0.14283274
   27    5    -0.00213    -0.95896    -6.08860     -0.00023930    0.99538612   -
0.00024041    0.14337410
   28    5    -0.97728    -2.45074    -4.75027     -0.00041769    0.49769306   -
0.00083926    0.13713110
   29    5    -1.70010    -1.88539    -4.95961     -0.00072618    1.16128380   -
0.00062533    0.13500813
   30    5    -1.12716    -1.02106    -5.85124     -0.00053264    1.16128380   -
0.00045867    0.13892000
   31    5     0.34685     0.34737    -6.35719     -0.00059331    1.16128380   -
0.00051091    0.14625758
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   32    5     1.21685     0.70869    -6.18261     -0.00068188    0.66359074   -
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   33    5    -0.43930     1.33936    -6.23274     -0.00068678    0.66359074   -
0.00103494    0.15049161
   34    5     1.25515    -0.02564    -6.14388     -0.00089122    0.82948843   -
0.00107443    0.15381709
   35    5    -0.83932    -1.80238    -5.47130     -0.00016718    0.66359074   -
0.00025193    0.13795240
   36    5     0.20617     1.39515    -6.25163     -0.00036320    0.66359074   -
0.00054733    0.15017329
   37    6    -1.19417    -1.20028     5.28442      0.00160840    1.16128380
0.00138502    0.08633233
   38    6    -0.15692    -5.94055     2.45370      0.00026238    0.33179537
0.00079080    0.08983675
   39    6    -0.25448    -6.07359     3.05892      0.00006587    0.16589769
0.00039704    0.08777855
   40    6    -1.98988    -0.83820     5.37579      0.00146612    0.99538612
0.00147291    0.08500566
   41    6    -6.05261    -1.44280     1.97448      0.00037143    0.66359074
0.00055972    0.09106659
   42    6    -2.28904    -2.61507     6.47482      0.00129615    0.82948843
0.00156259    0.07191034
   43    6    -1.88020    -1.83132     6.07808      0.00185975    1.16128380
0.00160146    0.07706999
   44    6     0.08879    -5.63034     2.48168      0.00009908    0.16589769
0.00059726    0.09301414
   45    6    -2.81276    -1.93599     6.30935      0.00074470    0.49769306
0.00149630    0.07410379
   46    6    -6.35097    -1.81541     2.36084      0.00015185    0.16589769
0.00091533    0.08670789
   47    7    -6.52645    -8.96444     1.87797      0.00122934    0.99538612
0.00123504    0.05643377
   48    7    -5.42316    -6.81612    -0.63777      0.00161498    1.16128380
0.00139068    0.06968199
   49    7    -7.39136    -3.35505     3.48304      0.00040924    0.49769306
0.00082228    0.07237002
   50    7    -7.84516    -3.92194     3.27920      0.00016868    0.16589769
0.00101677    0.07062572
   51    7    -4.82552    -7.44507    -0.49680      0.00159658    0.99538612
0.00160398    0.06921088
   52    7    -5.60913    -9.27708     1.61935      0.00098793    0.99538612
0.00099251    0.05982302
   53    7    -1.22348    -7.43868     3.43583      0.00043151    0.66359074
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   54    7    -1.55400    -7.71933     4.13181      0.00009197    0.16589769
0.00055437    0.07135443
   55    7    -6.53028    -8.46796     0.95322      0.00173879    1.32718149
0.00131014    0.05824043
   56    7    -5.92794    -7.71334    -0.09930      0.00160701    0.99538612
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   57    7    -7.27466    -8.21871     1.60467      0.00091107    0.82948843
0.00109835    0.05867058
   58    7    -7.41474    -3.32140     2.96046      0.00012598    0.16589769
0.00075936    0.07506620
   59    7    -5.83704    -8.43828     0.43693      0.00143545    0.99538612
0.00144210    0.06044238
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   60    7    -1.52536    -7.87547     3.74438      0.00014036    0.16589769
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0.00155349    0.15377803
   62    8     6.39129     2.22859     0.27106     -0.00135079    0.99538612   -
0.00135705    0.16731449
   63    8     5.21490     1.65648    -6.17914     -0.00124307    1.32718149   -
0.00093662    0.16049703
   64    8     5.83524     1.07828    -5.64984     -0.00172917    0.99538612   -
0.00173718    0.17037514
   65    8     6.62420     1.40802    -0.22861     -0.00166432    0.82948843   -
0.00200644    0.17663772
   66    8     5.81052     1.69774     0.47759     -0.00101169    0.99538612   -
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   67    8     5.44041     1.08992     0.36722     -0.00067095    0.49769306   -
0.00134813    0.16593537
   68    8     4.49071     0.79196    -5.90075     -0.00124336    1.16128380   -
0.00107067    0.16474467
   69    8     6.30278     2.04825    -5.77163     -0.00072368    0.99538612   -
0.00072704    0.16726788
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 1022   29    10.31444     6.58891    -5.53100     -0.00152770    0.52589089   -
0.00290497    0.14978992
 1023   29     9.67926     5.53253    -6.02150     -0.00148547    0.52589089   -
0.00282467    0.15282012
 1024   29     8.49595     5.09794    -6.43489     -0.00146903    0.52589089   -
0.00279342    0.15885511
 1025   29     7.23046     5.45627    -6.60840     -0.00170647    0.52589089   -
0.00324491    0.16477168
 1026   12     7.17013     9.08636    -5.08212     -0.00139696    0.51899348   -
0.00269167    0.15770954
 1027   12     8.60332     9.20163    -4.71558     -0.00120176    0.51899348   -
0.00231555    0.14920653
 1028   12     9.88432     8.45452    -4.66537     -0.00127834    0.51899348   -
0.00246312    0.14681491
 1029   12    10.50873     7.13920    -4.95128     -0.00134124    0.51899348   -
0.00258431    0.14725790
 1030   12    10.23066     5.77362    -5.46071     -0.00128059    0.51899348   -
0.00246745    0.14905103
 1031   12     9.15963     4.89548    -5.99308     -0.00114921    0.51899348   -
0.00221431    0.15423573
 1032   12     7.71735     4.85057    -6.33875     -0.00134309    0.51899348   -
0.00258788    0.16269517
 1033   12     6.63912     5.38258    -6.41261     -0.00075110    0.28804417   -
0.00260760    0.16488493
 1034   30     9.36744     2.87755    -3.99699     -0.00101546    0.25058321   -
0.00405240    0.17066304
 1035   30    10.26536     3.60372    -3.97172     -0.00157890    0.56179913   -
0.00281043    0.16111608
 1036   30    11.05402     4.48612    -3.23344     -0.00161573    0.56179913   -
0.00287600    0.15594853
 1037   30    11.17732     5.02244    -1.95171     -0.00184478    0.56179913   -
0.00328370    0.15474344
 1038   30    10.58090     4.97623    -0.69162     -0.00187790    0.56179913   -
0.00334265    0.15527016
 1039   30     9.52770     4.36786    -0.00873     -0.00173746    0.56179913   -
0.00309268    0.16044887
```

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 1040   30     8.63042     3.64103    -0.03744     -0.00087946    0.25058321   -
0.00350967    0.16868705
 1041   12     9.54500     3.33624    -4.34406     -0.00153685    0.54056524   -
0.00284304    0.16439430
 1042   12    10.66798     4.35662    -3.98398     -0.00150039    0.54056524   -
0.00277559    0.15428883
 1043   12    11.20842     5.19736    -2.78690     -0.00166566    0.54056524   -
0.00308133    0.15205420
 1044   12    10.92804     5.48781    -1.28059     -0.00164120    0.54056524   -
0.00303607    0.15138400
 1045   12     9.95046     5.09990    -0.12916     -0.00133248    0.54056524   -
0.00246497    0.15352810
 1046   12     8.70667     4.20466     0.15975     -0.00153850    0.54056524   -
0.00284609    0.16329217
 1047   31     6.89361     7.46572     0.75011     -0.00085314    0.24085526   -
0.00354213    0.16145645
 1048   31     7.96829     7.19991     0.85205     -0.00164868    0.53498145   -
0.00308176    0.15713598
 1049   31     9.24040     7.34182     0.43831     -0.00158488    0.53498145   -
0.00296249    0.15198892
 1050   31    10.00996     7.98173    -0.46053     -0.00170000    0.53498145   -
0.00317767    0.15038290
 1051   31     9.96400     8.85941    -1.47894     -0.00177155    0.53498145   -
0.00331143    0.15045141
 1052   31     9.12123     9.61796    -2.20278     -0.00168868    0.53498145   -
0.00315653    0.15170445
 1053   31     7.82436     9.94890    -2.33769     -0.00162444    0.53498145   -
0.00303645    0.15769683
 1054   12     7.17867     6.94983     0.78760     -0.00149362    0.52415054   -
0.00284959    0.15967334
 1055   12     8.67096     6.78942     0.68486     -0.00133486    0.52415054   -
0.00254672    0.15217610
 1056   12     9.87546     7.25066    -0.08951     -0.00123667    0.52415054   -
0.00235938    0.14838942
 1057   12    10.30236     8.14598    -1.22061     -0.00141380    0.52415054   -
0.00269731    0.14801938
 1058   12     9.77805     9.11130    -2.24847     -0.00153961    0.52415054   -
0.00293735    0.14838529
 1059   12     8.51574     9.75405    -2.75510     -0.00124683    0.52415054   -
0.00237876    0.15104571
 1060   12     7.30407     9.90269    -2.69321     -0.00069532    0.29194577   -
0.00238168    0.15749647
 1061   20     1.25847    -3.88515     3.09027      0.00002297    0.87083036
0.00002638    0.10611652
 1062   20     1.28267    -3.15548     3.95542     -0.00091019    1.74066732   -
0.00052290    0.10680181
 1063   20     0.66133    -2.11907     4.62036     -0.00066530    1.74066732   -
0.00038221    0.10297037
 1064   13     2.02989    -2.62795     2.57410     -0.00143647    1.74066732   -
0.00082524    0.12218350
 1065   13     1.79881    -1.64460     3.51325     -0.00157302    1.74066732   -
0.00090369    0.11947126
 1066   13     1.11827    -0.81910     3.88323     -0.00017897    0.87083036   -
0.00020552    0.11398238
 1067   23     5.16082    -0.59393    -0.67861     -0.00118672    0.86470476   -
0.00137239    0.17621727
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 1068   23     4.85688    -1.00139    -1.18664     -0.00166600    0.86470476   -
0.00192667    0.17879914
 1069   13     3.60786    -1.35434     0.35202     -0.00141831    1.72554404   -
0.00082195    0.15284342
 1070   19    -2.83921     0.37848     4.52275      0.00008953    0.87461797
0.00010237    0.09848476
 1071   19    -3.82178     0.68802     4.03779     -0.00090293    1.74828683   -
0.00051646    0.10315920
 1072   19    -4.73361     0.48146     3.01346     -0.00075928    1.74828683   -
0.00043430    0.10471706
 1073   14    -2.48604     1.50855     3.50722     -0.00118535    1.74828683   -
0.00067801    0.11459300
 1074   14    -3.61588     1.66579     2.71849     -0.00165670    1.74828683   -
0.00094761    0.11791428
 1075   14    -4.20471     1.31828     1.80802     -0.00028363    0.87461797   -
0.00032429    0.11752794
 1076   24    -3.29777     4.36242    -1.37901     -0.00172535    0.89572500   -
0.00192620    0.16044597
 1077   24    -2.91166     4.94797    -0.63179     -0.00355627    1.78824843   -
0.00198869    0.15721985
 1078   14    -3.30453     3.20090     0.06929     -0.00183282    1.78824843   -
0.00102492    0.14302564
 1079   14    -2.84290     3.76021     0.79343     -0.00065350    0.89572500   -
0.00072957    0.13986310
 1080   17     2.05947    -3.26997    -2.38922     -0.00100533    0.86185273   -
0.00116647    0.14998980
 1081   17     1.48314    -3.62509    -3.28674     -0.00303908    1.72273329   -
0.00176411    0.14730047
 1082   17     0.37221    -3.49183    -4.07792     -0.00283752    1.72273329   -
0.00164710    0.14243109
 1083   15     1.13112    -4.41102    -1.87924     -0.00146231    1.72273329   -
0.00084883    0.13040857
 1084   15     0.23729    -4.63317    -2.89395     -0.00163908    1.72273329   -
0.00095144    0.12661132
 1085   15    -0.73105    -4.34655    -3.38787     -0.00027433    0.86185273   -
0.00031831    0.12139996
 1086   21    -3.15754    -7.50216    -0.63481      0.00025293    0.87941181
0.00028762    0.08158153
 1087   21    -2.16587    -7.81926    -0.15341     -0.00064277    1.75793459   -
0.00036564    0.08692155
 1088   21    -1.24318    -7.61319     0.87444     -0.00062599    1.75793459   -
0.00035610    0.08864629
 1089   15    -2.04610    -6.65915    -1.32452     -0.00072412    1.75793459   -
0.00041191    0.09498452
 1090   15    -0.90454    -6.82240    -0.53682     -0.00099042    1.75793459   -
0.00056340    0.09889435
 1091   15    -0.30826    -6.47237     0.37839     -0.00002974    0.87941181   -
0.00003382    0.09826174
 1092   18    -3.30670    -1.09826    -4.47640     -0.00098123    0.85812334   -
0.00114346    0.13627910
 1093   18    -3.96403    -0.27980    -4.09166     -0.00298887    1.71523954   -
0.00174254    0.13993242
 1094   18    -4.17557     0.68827    -3.15540     -0.00282287    1.71523954   -
0.00164576    0.14382023
 1095   16    -4.30627    -1.78029    -3.49317     -0.00138455    1.71523954   -
0.00080721    0.12174163
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 1096   16    -4.90154    -0.75611    -2.81848     -0.00156268    1.71523954   -
0.00091106    0.12483146
 1097   16    -4.86610    -0.03894    -1.96151     -0.00026437    0.85812334   -
0.00030808    0.12541765
 1098   22    -7.23554    -3.24840     0.78902      0.00009268    0.87863039
0.00010548    0.08571430
 1099   22    -7.25389    -3.98822    -0.08748     -0.00073684    1.75638615   -
0.00041952    0.08697672
 1100   22    -6.61031    -5.03441    -0.75228     -0.00044215    1.75638615   -
0.00025174    0.08369012
 1101   16    -6.54160    -2.53250    -0.40355     -0.00083672    1.75638615   -
0.00047638    0.09744503
 1102   16    -6.29670    -3.52823    -1.35182     -0.00100678    1.75638615   -
0.00057321    0.09585006
 1103   16    -5.59485    -4.35921    -1.71624      0.00009900    0.87863039
0.00011267    0.09102081
 1104   23     4.74949    -1.35836    -2.34962     -0.00233916    0.82210254   -
0.00284534    0.18529921
 1105   23     4.90805    -1.30568    -3.40437     -0.00570723    1.64305201   -
0.00347355    0.18681790
 1106   23     4.85789    -0.87950    -4.38226     -0.00217399    0.82210254   -
0.00264443    0.18339068
 1107   17     3.49777    -2.05404    -2.98440     -0.00393160    1.64305201   -
0.00239286    0.17335801
 1108   17     3.56544    -1.75510    -4.25332     -0.00399616    1.64305201   -
0.00243215    0.17388837
 1109   24    -2.96305     4.43061    -4.23972     -0.00172032    0.95917683   -
0.00179353    0.16343920
 1110   24    -3.33035     4.19911    -3.10777     -0.00596626    1.91726739   -
0.00311186    0.16869233
 1111   18    -3.25758     2.84956    -4.16079     -0.00452557    1.91726739   -
0.00236043    0.16148539
 1112   18    -3.51537     2.60309    -3.00209     -0.00149868    0.95917683   -
0.00156246    0.15877009
 1113   27    -5.38754    -2.83070     7.26841      0.00033840    0.84724826
0.00039941    0.06874574
 1114   27    -6.31476    -2.55966     6.76276     -0.00042111    1.69325961   -
0.00024870    0.07361016
 1115   27    -7.16485    -2.76833     5.75983     -0.00051916    1.69325961   -
0.00030660    0.07437904
 1116   19    -4.98405    -1.69805     6.23917     -0.00022279    1.69325961   -
0.00013157    0.07896524
 1117   19    -6.04461    -1.57122     5.44469     -0.00057664    1.69325961   -
0.00034055    0.08194481
 1118   19    -6.59214    -1.90543     4.56298      0.00014534    0.84724826
0.00017154    0.08047090
 1119   28    -1.15193    -7.10618     5.90230      0.00010004    0.86269732
0.00011596    0.07392608
 1120   28    -1.13281    -6.38735     6.75068     -0.00059432    1.72422615   -
0.00034469    0.07585772
 1121   28    -1.73955    -5.36739     7.40720     -0.00025811    1.72422615   -
0.00014970    0.07246750
 1122   20    -0.37194    -5.84135     5.36941     -0.00046135    1.72422615   -
0.00026757    0.08335305
 1123   20    -0.60069    -4.87368     6.29177     -0.00055994    1.72422615   -
0.00032475    0.08223829
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 1124   20    -1.26379    -4.06048     6.66036      0.00024071    0.86269732
0.00027902    0.07712238
 1125   30     8.72907     2.13913    -1.20028     -0.00222196    0.94668561   -
0.00234709    0.17689047
 1126   30     9.05608     1.97615    -2.37378     -0.00540968    1.89288833   -
0.00285790    0.17928994
 1127   30     8.97916     2.22817    -3.57427     -0.00177758    0.94668561   -
0.00187768    0.17531531
 1128   23     7.82192     1.01385    -1.79059     -0.00677268    1.89288833   -
0.00357796    0.19017212
 1129   23     7.97785     1.06937    -3.27069     -0.00720478    1.89288833   -
0.00380624    0.19041398
 1130   31     6.65657    10.08348    -1.93277     -0.00105686    0.81227705   -
0.00130110    0.15998107
 1131   31     6.37659     9.84974    -0.98572     -0.00341271    1.62290950   -
0.00210284    0.16259750
 1132   25     5.03787    10.37611    -1.92565     -0.00450389    1.62290950   -
0.00277519    0.16829217
 1133   25     4.74637    10.06870    -1.00345     -0.00141332    0.81227705   -
0.00173995    0.16460254];
```

[PY] (Computation ID = 68)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.46
%   total number of segments         =    507
%   number of charge corr segments   =    235
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N             0.00000000000000    0.00000000000000   -2.52442218265784   3.4582  -
0.0536    20.43    -0.00263    5.9148
% C            -2.25650388834381    0.00000000000000   -1.30403950084875   3.7795  -
0.1063    55.35    -0.00192    6.2361
% C             2.25650388834381    0.00000000000000   -1.30403950084875   3.7795  -
0.1065    55.35    -0.00192    6.2361
% C            -2.29286756116516    0.00000000000000    1.31496407140523   3.7795  -
0.0497    47.82    -0.00104    6.2361
% C             2.29286756116516    0.00000000000000    1.31496407140523   3.7795  -
0.0497    47.82    -0.00104    6.2361
% C             0.00000000000000    0.00000000000000    2.63794552329561   3.7795  -
0.0579    49.20    -0.00118    6.2361
% H             0.00000000000000    0.00000000000000   -4.46564398266541   2.4566  -
0.1894    30.85    -0.00614    4.9133
% H            -3.94523815929033    0.00000000000000   -2.48310568739555   2.4566  -
0.0879    24.27    -0.00362    4.9133
% H             3.94523815929033    0.00000000000000   -2.48310568739555   2.4566  -
0.0879    24.27    -0.00362    4.9133
% H            -4.10566393974447    0.00000000000000    2.29698959243705   2.4566  -
0.0706    23.48    -0.00301    4.9133
% H             4.10566393974447    0.00000000000000    2.29698959243705   2.4566  -
0.0706    23.48    -0.00301    4.9133
% H             0.00000000000000    0.00000000000000    4.70250369083165   2.4566  -
0.0697    23.52    -0.00297    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -248.806224
%   Total energy + OC corr.      =       -248.802151
%   Dielectric energy            =         -0.097822      -2.662      -61.39
%   Diel. energy + OC corr.      =         -0.093750      -2.551      -58.83
%
%   Surface area of cavity [au]
acosmo =           425.823;
%   Total Volume of cavity [au]
vcosmo =           722.185;
```

```
%
%
% $screening_charge
%   cosmo           =   -1.02411
%   corrected total =   -0.99978
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1     0.02491     3.01136    -4.22452     -0.00202185    1.11114952   -
0.00181960    0.19652659
    2    1    -1.30769    -2.53036    -4.48561     -0.00089975    0.27778738   -
0.00323899    0.20997032
    3    1     1.06130    -2.54315    -4.61372     -0.00107358    0.41668107   -
0.00257650    0.21137383
    4    1     0.45543    -2.93962    -4.28803     -0.00185651    1.11114952   -
0.00167081    0.19871404
    5    1    -0.61520    -2.87359    -4.34735     -0.00175591    0.97225583   -
0.00180602    0.20072737
    6    1    -0.91395     2.79873    -4.33854     -0.00202153    0.97225583   -
0.00207921    0.20231579
    7    1     0.97780     2.74228    -4.39072     -0.00108881    0.55557476   -
0.00195979    0.20396288
    8    1     0.61943    -3.25737    -3.50674     -0.00032085    0.55557476   -
0.00057751    0.18558915
    9    1     0.04266    -3.45740    -2.58451     -0.00005643    0.69446845   -
0.00008126    0.17679818
   10    1    -0.32333     3.35797    -3.28518      0.00006541    0.69446845
0.00009418    0.18199891
   11    1     0.53949     3.23160    -3.63121     -0.00045860    0.69446845   -
0.00066036    0.18685554
   12    1     0.08065     3.45608    -2.61533     -0.00018230    0.69446845   -
0.00026250    0.17698430
   13    1    -0.34064    -3.29914    -3.50354     -0.00068597    1.11114952   -
0.00061735    0.18450301
   14    2    -1.26601     3.63418    -0.99415     -0.00061970    0.66359074   -
0.00093386    0.16460226
   15    2    -4.64754     2.91383    -1.02670     -0.00043446    1.16128380   -
0.00037412    0.16279496
   16    2    -2.79349     2.55807    -4.03391     -0.00203479    0.99538612   -
0.00204423    0.19268111
   17    2    -3.65531    -3.40392    -2.16475     -0.00128743    1.32718149   -
0.00097005    0.16503248
   18    2    -4.48119    -2.79182    -2.54525     -0.00223216    1.32718149   -
0.00168188    0.17362609
   19    2    -3.31362    -1.70642    -4.50634     -0.00066486    0.49769306   -
0.00133589    0.20562607
   20    2    -3.38530     1.99148    -4.31137     -0.00247752    0.99538612   -
0.00248901    0.19918546
   21    2    -5.01517     2.54264    -1.76131     -0.00172903    0.99538612   -
0.00173704    0.17109932
   22    2    -5.89731    -0.85729    -0.76200     -0.00231696    0.82948843   -
0.00279324    0.18150664
   23    2    -1.13366    -3.60302    -1.10000     -0.00069026    0.66359074   -
0.00104019    0.16631654
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  497    6     2.14057     0.97484     5.53712     -0.00189565    0.52187097   -
0.00363241    0.16663831
  498    6     1.10733     2.07515     5.53711     -0.00174504    0.52187097   -
0.00334381    0.15920704
  499    6    -0.38191     2.32091     5.53709     -0.00175296    0.52187097   -
0.00335898    0.15744817
```

```
  500    6    -1.71389     1.61092     5.53708     -0.00155421    0.52187097   -
0.00297815    0.16232039
  501    6    -2.36069     0.56849     5.53707     -0.00105225    0.29132383   -
0.00361195    0.16632732
  502    8    -3.51579     0.47122    -5.04288     -0.00315210    0.87076341   -
0.00361993    0.21218851
  503    8    -3.51578    -0.47126    -5.04287     -0.00296969    0.87076341   -
0.00341044    0.21223081
  504    7    -2.29660    -0.00001    -5.62144     -0.01047399    1.74228297   -
0.00601164    0.23431375
  505    9     3.51575    -0.47130    -5.04288     -0.00315698    0.87084113   -
0.00362521    0.21218295
  506    9     3.51576     0.47127    -5.04288     -0.00295264    0.87084113   -
0.00339056    0.21222765
  507    7     2.29658    -0.00000    -5.62143     -0.01040771    1.74243948   -
0.00597307    0.23433641];
```

[EPY] (Computation ID = 69)

```
% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.46
%   total number of segments         =    660
%   number of charge corr segments   =    302
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N            -0.15100655378495   -0.35773168068560    0.62906442153234   3.4582  -
0.0071     3.21    -0.00220    5.9148
% C            -1.50148304146215   -2.85025955618873    0.52845842242003   3.7795  -
0.0413    25.90    -0.00159    6.2361
% C             2.41687434937355   -0.29296081886374    0.62262489630251   3.7795  -
0.0772    46.38    -0.00167    6.2361
% C            -1.51107003783399    1.82130076150286    0.63613925378814   3.7795  -
0.0745    44.29    -0.00168    6.2361
% C            -2.10270329907495   -3.64145485231088   -2.17592053002294   3.7795  -
0.0177    60.36    -0.00029    6.2361
% C             3.70386725477551    1.99093156224028    0.63216767119330   3.7795  -
0.0464    47.66    -0.00097    6.2361
% C            -0.31081346586296    4.15094103859697    0.64823272809011   3.7795  -
0.0468    48.34    -0.00097    6.2361
% C             2.33020438879330    4.24859201249639    0.64627740768160   3.7795  -
0.0550    49.77    -0.00110    6.2361
% H            -3.21483618384203   -2.63906866829874    1.67779281473170   2.4566  -
0.0668    23.32    -0.00286    4.9133
% H            -0.27845936094201   -4.22465870671239    1.48537896938475   2.4566  -
0.0669    22.94    -0.00292    4.9133
% H             3.36897936583545   -2.11864238504354    0.61654494815974   2.4566  -
0.0839    23.27    -0.00361    4.9133
% H            -3.55925845350943    1.61317369413823    0.64314761303776   2.4566  -
0.0833    23.15    -0.00360    4.9133
% H            -3.07958604732954   -5.47551556050493   -2.12959849555184   2.4566  -
0.0432    24.26    -0.00178    4.9133
% H            -0.37631500162940   -3.86386212457810   -3.31114694707106   2.4566  -
0.0405    23.39    -0.00173    4.9133
% H            -3.35179268446388   -2.27388697669140   -3.11963490926658   2.4566  -
0.0412    22.95    -0.00179    4.9133
% H             5.76578732754369    1.97871209233865    0.63843796200001   2.4566  -
0.0704    23.50    -0.00299    4.9133
% H            -1.45442874945597    5.86687788067536    0.67002318082440   2.4566  -
0.0704    23.51    -0.00299    4.9133
% H             3.30604019286984    6.06751228788933    0.66201059276607   2.4566  -
0.0676    23.14    -0.00292    4.9133
% $end
```

```
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                 =       -327.442484
%   Total energy + OC corr.      =       -327.438180
%   Dielectric energy            =         -0.085295      -2.321      -53.52
%   Diel. energy + OC corr.      =         -0.080990      -2.204      -50.82
%
%   Surface area of cavity [au]
acosmo =           559.340;
%   Total Volume of cavity [au]
vcosmo =          1025.140;
%
%
% $screening_charge
%   cosmo           =   -1.02906
%   corrected total =   -1.00007
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1    -0.14847    -0.18653     4.08302     -0.00005383    0.13889369   -
0.00038759    0.16567005
    2    1     0.01654    -0.99428     4.02404     -0.00026995    0.13889369   -
0.00194355    0.16925687
    3    1    -0.28545    -0.52893     4.08040     -0.00023210    0.27778738   -
0.00083553    0.16680823
    4    2    -3.38810    -5.89075     1.74513     -0.00110109    0.99538612   -
0.00110619    0.14798809
    5    2    -1.52365    -3.96792     4.13882     -0.00070547    1.16128380   -
0.00060749    0.15495435
    6    2    -2.36674    -3.72189     4.10281     -0.00062771    0.99538612   -
0.00063062    0.15549071
    7    2    -3.55028    -5.37452     2.45583     -0.00103098    0.99538612   -
0.00103576    0.15041025
    8    2    -4.15932    -5.34100     1.53659     -0.00072098    0.66359074   -
0.00108648    0.15116123
    9    2    -2.45446    -5.80178     2.68822     -0.00095508    1.16128380   -
0.00082244    0.14974692
   10    2    -2.10789    -4.90895     3.63947     -0.00058296    1.16128380   -
0.00050199    0.15151431
   11    2    -1.45165    -2.92333     4.30689     -0.00060477    0.99538612   -
0.00060757    0.15858461
   12    2    -1.42988    -1.88013     4.18060     -0.00092459    0.66359074   -
0.00139332    0.16586066
   13    2    -2.39127    -6.32378     1.72307     -0.00150124    1.16128380   -
0.00129274    0.14971783
   14    2    -0.44612    -3.15615     4.14467     -0.00099291    0.82948843   -
0.00119702    0.16382207
   15    2    -2.10185    -2.18065     4.19937     -0.00098635    0.82948843   -
0.00118910    0.16498252
   16    2    -2.90599    -5.07947     3.23812     -0.00072059    0.99538612   -
0.00072393    0.15031950
   17    2    -4.62256    -4.91233     1.06785     -0.00050051    0.33179537   -
0.00150848    0.15369254
```

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   18    2    -1.71383    -6.57000     1.16296     -0.00043448    0.49769306   -
0.00087299    0.15301177
   19    2    -0.61996    -2.47649     4.18463     -0.00078906    0.66359074   -
0.00118908    0.16451634
   20    3     1.69108     0.43245     4.26012     -0.00062976    0.66359074   -
0.00094902    0.15465738
   21    3     4.67270    -1.15817     3.52898     -0.00027731    1.16128380   -
0.00023880    0.15502388
   22    3     3.82049    -1.65714    -2.61049     -0.00114507    0.99538612   -
0.00115038    0.15763536
   23    3     4.20187    -2.21599    -2.09765     -0.00128068    0.82948843   -
0.00154394    0.16516604
   24    3     4.65815    -1.97878     3.15619     -0.00151922    0.99538612   -
0.00152626    0.16357618
   25    3     5.88191    -1.54269    -0.22344     -0.00231435    0.66359074   -
0.00348761    0.17529523
   26    3     1.58137     0.50519    -2.97586     -0.00068431    0.49769306   -
0.00137496    0.15645350
   27    3     5.41539    -1.57201     2.53500     -0.00124123    0.66359074   -
0.00187047    0.16646349
   28    3     3.78158    -1.71259     3.84854     -0.00099987    1.16128380   -
0.00086100    0.15657455
   29    3     2.50060    -2.30447     3.82125     -0.00109416    0.99538612   -
0.00109924    0.16586541
   30    3     4.61384    -1.10215    -2.34430     -0.00083370    0.99538612   -
0.00083756    0.15518806
   31    3     5.31167    -1.33354    -1.57315     -0.00010510    0.66359074   -
0.00015838    0.16275535
   32    3     3.72888    -0.66392     4.14758     -0.00049022    1.16128380   -
0.00042213    0.14936113
   33    3     2.59136    -0.04174     4.38969     -0.00005750    1.16128380   -
0.00004952    0.14959918
   34    3     1.59789    -0.33543     4.31205     -0.00053623    0.66359074   -
0.00080807    0.15696173
   35    3     1.85885    -1.28400     4.22691     -0.00152207    1.16128380   -
0.00131067    0.16026724
   36    3     3.52116    -0.54210    -2.98329     -0.00057985    1.65897686   -
0.00034953    0.15048182
   37    3     3.33879    -2.60172     3.46938     -0.00220405    1.16128380   -
0.00189794    0.16800082
   38    3     5.75880    -1.58610     1.82408     -0.00060351    0.33179537   -
0.00181893    0.17270740
   39    3     5.13031    -1.87477    -1.47958     -0.00146337    0.82948843   -
0.00176418    0.16752030
   40    3     2.34977     0.23264    -3.11949     -0.00089841    1.16128380   -
0.00077364    0.15150237
   41    3     2.75988    -1.19825     4.27600     -0.00114778    1.32718149   -
0.00086483    0.15444184
   42    4    -0.53289     1.82378    -3.01454     -0.00042039    0.33179537   -
0.00126703    0.15377039
   43    4    -3.43404     3.29724    -2.26354     -0.00007612    0.99538612   -
0.00007647    0.15559810
   44    4    -3.13274     1.92255     4.04849     -0.00083580    0.99538612   -
0.00083968    0.15583219
   45    4    -4.04874     1.81671     3.43694     -0.00215628    1.32718149   -
0.00162471    0.16610006
```

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   46    4    -4.17172     2.96371    -1.79289     -0.00099317    0.66359074   -
0.00149667    0.16433121
   47    4    -4.45934     4.02896     1.48357     -0.00199431    0.66359074   -
0.00300533    0.17535700
   48    4    -0.41817     1.44933     4.23494     -0.00067105    0.66359074   -
0.00101124    0.15635919
   49    4    -4.22867     3.62314    -1.27496     -0.00145750    0.66359074   -
0.00219639    0.16674307
   50    4    -3.69433     2.40544    -2.39314     -0.00163317    1.32718149   -
0.00123055    0.15948810
   51    4    -3.36333     0.97049     3.81883     -0.00134194    1.16128380   -
0.00115557    0.16533199
   52    4    -3.48848     3.01054     3.62943     -0.00137598    1.49307918   -
0.00092157    0.15523350
   53    4    -3.97055     3.66756     2.83307     -0.00021216    0.66359074   -
0.00031971    0.16266664
   54    4    -2.44341     2.84798    -2.87968     -0.00042370    0.99538612   -
0.00042566    0.14987562
   55    4    -1.27426     2.20764    -3.11606     -0.00007881    0.82948843   -
0.00009501    0.15019197
   56    4    -1.37242     0.90099     4.29920     -0.00082573    0.82948843   -
0.00099547    0.15885066
   57    4    -2.21101     1.19395     4.29684     -0.00177182    1.49307918   -
0.00118669    0.15724872
   58    4    -2.37259     2.57110     4.23888     -0.00014061    1.49307918   -
0.00009417    0.14933207
   59    4    -4.42888     3.90226    -0.56396     -0.00031897    0.33179537   -
0.00096135    0.17313225
   60    4    -4.32303     3.21856     2.73965     -0.00080423    0.82948843   -
0.00096956    0.16727843
   61    4    -1.17459     1.97294     4.39752     -0.00053335    1.16128380   -
0.00045928    0.15052862
   62    4    -2.31219     2.24804    -3.03271     -0.00077394    0.66359074   -
0.00116629    0.15191864
   63    5    -5.68996    -3.89255    -3.33899      0.00054544    0.82948843
0.00065756    0.12112332
   64    5    -2.55799    -5.25165    -5.56478      0.00037819    1.32718149
0.00028496    0.11027712
   65    5    -0.19436    -6.77313    -3.08983      0.00078764    1.32718149
0.00059347    0.12400853
   66    5    -1.40346    -0.75145    -4.50900      0.00015924    0.66359074
0.00023997    0.13852756
   67    5    -1.03274    -7.18502    -2.93927      0.00039978    0.99538612
0.00040163    0.12226601
   68    5    -3.03269    -6.06119    -4.92626      0.00003753    1.49307918
0.00002514    0.11285212
   69    5    -5.66915    -4.63373    -2.93753      0.00063613    1.32718149
0.00047931    0.12071575
   70    5    -5.20014    -4.97144    -0.46679     -0.00027354    0.66359074   -
0.00041222    0.14052654
   71    5    -1.62512    -1.87228    -5.48141      0.00088250    1.32718149
0.00066494    0.12502657
   72    5    -0.93040    -2.06406    -5.40422      0.00042701    0.82948843
0.00051479    0.12715627
   73    5    -5.68157    -4.02019    -1.02161      0.00016093    0.99538612
0.00016168    0.13535173
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   74    5    -5.88143    -3.59545    -2.11880     0.00068535    1.32718149
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   75    5    -5.09961    -4.42793    -4.34025     0.00100459    1.82487455
0.00055050    0.11515980
   76    5    -3.83929    -4.95243    -5.26622     0.00053413    1.49307918
0.00035774    0.11056789
   77    5    -1.57552    -5.92059    -5.14443     0.00057197    1.49307918
0.00038308    0.11341472
   78    5    -0.85194    -6.64049    -4.10614     0.00079557    1.16128380
0.00068508    0.11756384
   79    5    -0.45831    -7.03001    -1.86289     0.00049044    1.16128380
0.00042232    0.12976741
   80    5    -0.47925    -6.86061    -1.04201     0.00026670    0.49769306
0.00053588    0.13843574
   81    5    -2.66071    -2.97614    -5.85428     0.00035224    1.32718149
0.00026541    0.11773901
   82    5    -2.86355    -4.13550    -5.84490     0.00047588    1.65897686
0.00028685    0.11185608
   83    5    -1.65744    -4.67340    -5.78442     0.00016126    1.16128380
0.00013886    0.11491657
   84    5     0.48077    -6.39763    -2.29233     0.00023719    0.99538612
0.00023829    0.13479523
   85    5     0.98160    -5.75042    -1.60698    -0.00037556    0.49769306   -
0.00075459    0.15008998
   86    5    -0.61672    -1.13069    -4.57847     0.00060081    1.49307918
0.00040239    0.13702662
   87    5    -1.21879    -7.12748    -1.01377    -0.00034431    0.66359074   -
0.00051886    0.13753654
   88    5    -1.78067    -6.62767    -4.47009     0.00049686    1.16128380
0.00042786    0.11444942
   89    5    -4.48207    -5.26836    -4.62053     0.00021397    0.99538612
0.00021496    0.11342741
   90    5    -5.72327    -4.58104    -1.63476     0.00016274    0.82948843
0.00019619    0.12886282
   91    5    -1.62593    -3.34788    -5.91369     0.00049018    1.49307918
0.00032830    0.11801578
   92    5    -5.70154    -2.77438    -1.41388    -0.00002680    1.16128380   -
0.00002307    0.14184193
   93    5    -4.07696    -3.85391    -5.39174     0.00010839    1.32718149
0.00008167    0.11520813
   94    5     0.42135    -6.37845    -1.52606     0.00006047    0.82948843
0.00007290    0.14045353
   95    6     2.78404     2.04666     4.29755     0.00035110    0.49769306
0.00070546    0.14037651
   96    6     5.50607     3.56929     3.55539    -0.00012791    1.16128380   -
0.00011015    0.14029128
   97    6     5.78744     0.42729     3.37042    -0.00053359    0.99538612   -
0.00053607    0.14834759
   98    6     5.35452     2.08457    -2.76650    -0.00026467    1.32718149   -
0.00019942    0.13751377
   99    6     6.14822     2.48534    -2.20774    -0.00079084    1.16128380   -
0.00068100    0.14332563
  100    6     6.36656    -0.16931    -0.95772    -0.00028620    0.33179537   -
0.00086259    0.16340045
  101    6     6.33409     0.15083     2.62723    -0.00086683    0.99538612   -
0.00087085    0.15794863
```

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  102    6     6.22684     3.17406     3.18544     -0.00094360    0.99538612   -
0.00094797    0.14539235
  103    6     6.43403     4.47241    -0.18813     -0.00077024    0.66359074   -
0.00116072    0.15921116
  104    6     6.22516     4.03595     2.56747     -0.00077442    0.66359074   -
0.00116702    0.15049045
  105    6     5.57746     2.52114     3.87144     -0.00028446    1.16128380   -
0.00024495    0.13800318
  106    6     5.56905     1.19476     3.82145     -0.00021636    0.82948843   -
0.00026083    0.14113708
  107    6     6.18704     0.31622    -1.67293     -0.00110055    0.99538612   -
0.00110565    0.15407224
  108    6     5.49913     0.78981    -2.46922     -0.00000433    1.32718149   -
0.00000327    0.14399357
  109    6     5.54280     3.44128    -2.33417     -0.00016206    1.32718149   -
0.00012211    0.13983508
  110    6     5.99062     4.07128    -1.54207     -0.00054504    0.66359074   -
0.00082134    0.14748613
  111    6     4.59635     2.79840     4.21487      0.00012151    1.16128380
0.00010464    0.13477960
  112    6     3.63788     2.32465     4.39628      0.00045735    0.82948843
0.00055137    0.13533874
  113    6     3.68720     1.58597     4.38982      0.00035501    0.82948843
0.00042799    0.13751140
  114    6     4.69319     0.89219     4.11042      0.00052039    0.99538612
0.00052280    0.14033740
  115    6     4.36516     1.40590    -3.04271      0.00034509    1.82487455
0.00018910    0.13812322
  116    6     4.51345     2.83309    -2.96223      0.00020063    1.49307918
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  587    6     6.61147     3.85858     2.05188     -0.00175379    0.51182657   -
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  588    6     6.60169     2.64278     2.89833     -0.00159106    0.51182657   -
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  589    6     6.59306     1.16210     2.85103     -0.00154775    0.51182657   -
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  590    6     6.58899     0.00278     1.92870     -0.00189355    0.51182657   -
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  591    8     1.35176     3.33692    -2.89252     -0.00021662    0.62354631   -
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  593    8     1.21596     7.03908    -1.47708     -0.00247604    1.26736949   -
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  597    8     1.35845     3.29814     4.17672     -0.00024977    0.62354631   -
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  598    7     0.70085     4.02112    -2.88682     -0.00083907    1.26736949   -
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  599    7     0.62110     6.19098    -2.26841     -0.00157355    1.26736949   -
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  605   17    -3.17545     6.09750     2.33494     -0.00182335    0.52052265   -
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  612   17    -3.19641     6.12549    -0.96874     -0.00165212    0.52052265   -
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  613   17    -3.77423     5.72972    -0.12871     -0.00095935    0.23481795   -
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  624   18     2.76635     7.68974    -1.03407     -0.00195053    0.51043940   -
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  625   18     2.08854     8.04425     0.02183     -0.00169880    0.51043940   -
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  628   18     3.85013     7.07531     2.78048     -0.00161342    0.51043940   -
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  629   18     4.94379     6.49207     2.37581     -0.00168724    0.51043940   -
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  631   18     5.62465     6.14720     0.01609     -0.00199861    0.51043940   -
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  642    8     5.38643     5.91114    -0.72139     -0.00178978    0.50573360   -
0.00353898    0.15813920
  643    8     4.34869     6.47527    -1.57694     -0.00159557    0.50573360   -
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  644   12    -5.53808    -0.13696     0.57743     -0.00248369    0.76078935   -
0.00326462    0.18322755
  645   12    -5.43745     0.12759     1.63123     -0.00555712    1.52150195   -
0.00365239    0.18450920
  646   12    -4.91854     0.39399     2.55339     -0.00206532    0.76078935   -
0.00271470    0.18123445
  647    9    -5.42154    -1.33634     1.29805     -0.00436713    1.52150195   -
0.00287027    0.17770703
  648    9    -5.03498    -1.00506     2.53095     -0.00447883    1.52150195   -
0.00294369    0.17880141
  649   11     3.11503    -3.96544     2.47092     -0.00250242    0.83790819   -
0.00298651    0.18213020
  650   11     3.20051    -4.55066     1.41119     -0.00642177    1.67673305   -
0.00382993    0.18618619
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0.00351352    0.18407784
  652   10     2.05316    -4.85647     2.34503     -0.00538891    1.67673305   -
0.00321393    0.18057645
  653   10     1.98085    -5.30939     0.94353     -0.00501166    1.67673305   -
0.00298894    0.17958114
  654   14     2.31341    -4.20718    -2.89562     -0.00107716    1.03341970   -
0.00104233    0.15551737
  655   14     1.99707    -4.81961    -2.32184     -0.00083706    1.03341970   -
0.00080999    0.15603794
  656   11     3.31851    -3.93897    -1.35427     -0.00531050    2.06290961   -
0.00257428    0.17621938
  657   15    -5.41882    -0.98340    -1.89179     -0.00057983    0.84458968   -
0.00068652    0.15683756
  658   15    -5.09606    -0.30771    -2.57200     -0.00258508    1.68692718   -
0.00153242    0.15763544
  659   12    -5.38443     0.49572    -0.97806     -0.00433372    1.68692718   -
0.00256900    0.17601794
  660   12    -4.98759     1.15380    -1.63598     -0.00129595    0.84458968   -
0.00153442    0.17119394];
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[BMPYR] (Computation ID = 699)

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% COSMO Results from DMol3
%
% Note: COSMO for ideal conductor limit (fepsi= 1.0000)
%   Basic Grid Size                  =   1082
%   Number of Segments on an Atom    =     92
%   Number of Segments on Hydrogen   =     32
%   Solvent Radius    [au]           =   2.46
%   A - Matrix Cutoff [au]           =  13.23
%   factor for Outlying Charge corr  =   0.85
%   maximum segment or cutoff radius =   1.46
%   total number of segments         =    780
%   number of charge corr segments   =    330
%
%
%
%
% $coordinates xyz [au]                          and cosmo atom analysis:   radius
charge    area  charge density  (srad)
% N             0.31652781626624   -0.17564515846611    0.03759609567756   3.4582  -
0.0130     6.21    -0.00210    5.9148
% C             0.28448919923213   -3.02069851351131    0.05226072945547   3.7795  -
0.0474    26.36    -0.00180    6.2361
% C            -1.94622673280022    1.10964264894300    0.02559642171125   3.7795  -
0.0377    23.48    -0.00160    6.2361
% C             2.55321461200079    1.09273387090535    0.06124928735805   3.7795  -
0.0677    46.82    -0.00145    6.2361
% C            -1.88737797974655    3.74716660030512    0.02703232443815   3.7795  -
0.0333    45.90    -0.00073    6.2361
% C             2.84332599409888   -4.30304095598748   -0.17958796980072   3.7795  -
0.0157    50.67    -0.00031    6.2361
% C            -4.38169156140013   -0.32540389596010    0.01735141434708   3.7795  -
0.0369    51.26    -0.00072    6.2361
% C             2.65287573671225    3.70610319931861    0.06764108188542   3.7795  -
0.0363    48.24    -0.00075    6.2361
% C             0.39255756240586    5.06733518228896    0.04701163719808   3.7795  -
0.0450    49.03    -0.00092    6.2361
% H            -0.94986101780107   -3.59376163454320   -1.51385173927142   2.4566  -
0.0580    20.33    -0.00285    4.9133
% H            -0.65284419471757   -3.57922475758969    1.82085993573104   2.4566  -
0.0621    22.29    -0.00279    4.9133
% H             4.25066382876135   -0.06130530639930    0.07763894440108   2.4566  -
0.0533    14.66    -0.00364    4.9133
% H            -3.68524401891650    4.75609985953004    0.01351946550534   2.4566  -
0.0648    22.61    -0.00287    4.9133
% H             3.83974978605103   -3.79414347608111   -1.93123656328168   2.4566  -
0.0455    23.44    -0.00194    4.9133
% H             2.49789112224631   -6.35114531097570   -0.24841386830254   2.4566  -
0.0456    24.22    -0.00188    4.9133
% H             4.07634629747435   -3.95502181940829    1.45604186522467   2.4566  -
0.0461    23.34    -0.00197    4.9133
% H            -4.54213290556090   -1.59485985757348    1.65927423578994   2.4566  -
0.0529    21.97    -0.00241    4.9133
% H            -4.58468873287243   -1.49188869614039   -1.69582461156201   2.4566  -
0.0541    22.00    -0.00246    4.9133
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% H            -5.97234898356590    0.99944613478880    0.07260039220045   2.4566  -
0.0518    22.39    -0.00231    4.9133
% H             4.49208907987309    4.63636948621291    0.08490708619083   2.4566  -
0.0674    23.51    -0.00287    4.9133
% H             0.40268509225904    7.13124240034333    0.04833383510404   2.4566  -
0.0654    23.14    -0.00283    4.9133
% $end
%
%
% $cosmo_energy               [Hartree atomic units]       [eV]     [kcal/mol]
%   Total energy                =       -366.767162
%   Total energy + OC corr.     =       -366.762705
%   Dielectric energy           =         -0.081699      -2.223      -51.27
%   Diel. energy + OC corr.     =         -0.077242      -2.102      -48.47
%
%   Surface area of cavity [au]
acosmo =           611.881;
%   Total Volume of cavity [au]
vcosmo =          1149.013;
%
%
% $screening_charge
%   cosmo           =   -1.03114
%   corrected total =   -1.00018
%
%
% $segment information
%     n  atom        position (X, Y, Z) [au]            charge       area [au]
charge/area    potential [au]
%
data = [1    1     0.38863    -0.44686    -3.40920     -0.00036181    0.41668107   -
0.00086831    0.16478087
    2    1     0.20026    -0.03860     3.49112     -0.00009177    0.13889369   -
0.00066075    0.16383487
    3    1     0.24080    -0.40513     3.48734     -0.00044708    0.27778738   -
0.00160943    0.16632897
    4    1     0.20957     0.01335    -3.41378     -0.00007323    0.13889369   -
0.00052724    0.16241780
    5    2     0.76301    -1.94376    -3.53876     -0.00084874    0.49769306   -
0.00170536    0.16571295
    6    2    -1.22694    -6.48279     0.16902     -0.00081964    0.82948843   -
0.00098813    0.15018504
    7    2     1.40198    -2.59800     3.63792     -0.00066182    0.49769306   -
0.00132977    0.16348879
    8    2    -1.42662    -6.28147    -0.79838     -0.00103994    0.99538612   -
0.00104476    0.15370339
    9    2     0.03984    -2.09213    -3.60315     -0.00112513    0.66359074   -
0.00169551    0.16893015
   10    2    -1.93225    -6.03174     0.60353     -0.00088604    1.16128380   -
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   11    2    -2.63377    -5.35406     0.62094     -0.00091194    0.82948843   -
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0.00162977    0.16768379
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   16    2    -0.49427    -6.33960     1.68401     -0.00060021    0.49769306   -
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   20    3    -2.35091     0.94427    -3.72848     -0.00087192    0.82948843   -
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   21    3    -2.01705     1.66868    -3.71160      0.00053486    0.66359074
0.00080601    0.14729610
   22    3    -0.81104     1.54175    -3.55334     -0.00052933    0.49769306   -
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   23    3    -1.26780     1.39932     3.73237     -0.00131139    1.49307918   -
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   25    3    -2.69882     1.51070     3.70760     -0.00037074    1.32718149   -
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   26    3    -1.21200     0.94606    -3.67822     -0.00119754    0.99538612   -
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   27    4     1.52203     1.38764     3.68532     -0.00055020    0.66359074   -
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   28    4     4.86735     1.35103     3.03819     -0.00018827    1.32718149   -
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   29    4     4.07462     0.41012    -3.33046     -0.00084531    0.99538612   -
0.00084923    0.14937924
   30    4     5.05249     0.50291    -2.71184     -0.00144024    0.99538612   -
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   31    4     5.29136     0.66804     2.63153     -0.00137267    0.99538612   -
0.00137903    0.15642262
   32    4     6.20806     1.63193    -0.73599     -0.00139938    0.66359074   -
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   34    4     5.77415     1.38486     2.01685     -0.00128773    0.66359074   -
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   36    4     3.30692    -0.12796     3.55783     -0.00114646    0.82948843   -
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   37    4     4.87179     1.35051    -2.91231     -0.00071835    1.16128380   -
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   44    4     2.90754     0.50548    -3.65546     -0.00085421    1.16128380   -
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   47    4     5.79136     1.01226    -1.88611     -0.00093991    0.66359074   -
0.00141639    0.16089667
   48    4     2.29537     1.52458    -3.68459     -0.00031058    1.16128380   -
0.00026744    0.14345470
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0.00180903    0.14160003
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0.00242574    0.14429040
  691   19    -6.40482     2.19521     2.17328     -0.00060449    0.24660897   -
0.00245122    0.14928554
  692    7    -6.51604     1.73205    -2.24745     -0.00117666    0.53386253   -
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  693    7    -7.46387     0.57872    -1.88018     -0.00106919    0.53386253   -
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0.00226344    0.13731228
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0.00218744    0.14557564
  698    9     0.76638     3.78938     3.58808     -0.00005823    0.62102787   -
0.00009377    0.13403540
  699    9     1.71694     5.36595     3.46724     -0.00082446    1.26211643   -
0.00065324    0.13071837
  700    9     2.68953     6.96186     2.20937     -0.00219380    1.26211643   -
0.00173819    0.14285319
  701    9     3.08108     7.57970     0.07862     -0.00364766    1.26211643   -
0.00289012    0.15642061
  702    9     2.73295     6.96915    -2.06175     -0.00215824    1.26211643   -
0.00171002    0.14294027
  703    9     1.78618     5.37758    -3.34458     -0.00081393    1.26211643   -
0.00064489    0.13079672
  704    9     0.83833     3.80146    -3.49009     -0.00011116    0.62102787   -
0.00017899    0.13402158
  705    8     1.66536     4.07225     3.59356     -0.00051159    1.26211643   -
0.00040534    0.13205236
  706    8     2.78993     5.93053     2.99585     -0.00129511    1.26211643   -
0.00102614    0.13472317
  707    8     3.50941     7.09812     1.20861     -0.00327053    1.26211643   -
0.00259130    0.15185066
  708    8     3.53231     7.10196    -1.04407     -0.00293518    1.26211643   -
0.00232560    0.15199985
  709    8     2.84935     5.94051    -2.84955     -0.00127874    1.26211643   -
0.00101317    0.13479843
  710    8     1.73722     4.08432    -3.47633     -0.00049956    1.26211643   -
0.00039581    0.13192190
  711   20     6.44157     3.37872    -0.72538     -0.00092899    0.23405005   -
0.00396919    0.16122682
  712   20     6.13097     4.00829    -1.56075     -0.00168239    0.51864554   -
0.00324381    0.15591271
  713   20     5.57341     5.11896    -2.00948     -0.00162654    0.51864554   -
0.00313613    0.15017194
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  714   20     4.99945     6.24669    -1.62917     -0.00184109    0.51864554   -
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0.00325771    0.15504419
  716   20     4.62428     6.94430     0.75159     -0.00198891    0.51864554   -
0.00383481    0.15501252
  717   20     4.97090     6.23933     1.81400     -0.00167898    0.51864554   -
0.00323724    0.15080289
  718   20     5.53851     5.10997     2.19895     -0.00177704    0.51864554   -
0.00342631    0.15019398
  719   20     6.10348     4.00120     1.75479     -0.00151413    0.51864554   -
0.00291940    0.15583327
  720   20     6.42791     3.37520     0.92200     -0.00093244    0.23405005   -
0.00398393    0.16122024
  721    8     6.13686     3.26980    -1.20964     -0.00171462    0.51030599   -
0.00335999    0.16035951
  722    8     5.61911     4.31035    -2.12240     -0.00145641    0.51030599   -
0.00285398    0.14931381
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0.00294649    0.14626386
  724    8     4.40009     6.70552    -1.31465     -0.00151567    0.51030599   -
0.00297012    0.15129153
  725    8     4.17912     7.11641     0.08760     -0.00197112    0.51030599   -
0.00386263    0.15603323
  726    8     4.37682     6.69952     1.49155     -0.00162451    0.51030599   -
0.00318341    0.15116385
  727    8     4.91528     5.61912     2.34403     -0.00148770    0.51030599   -
0.00291531    0.14622171
  728    8     5.58236     4.30088     2.30916     -0.00144351    0.51030599   -
0.00282872    0.14933214
  729    8     6.11522     3.26422     1.40067     -0.00172971    0.51030599   -
0.00338955    0.16032914
  730   21     0.64959     8.29037     2.20195     -0.00069679    0.23109267   -
0.00301521    0.14510236
  731   21     1.63345     8.28582     1.76645     -0.00187521    0.51031059   -
0.00367464    0.14940964
  732   21     2.40891     8.28269     0.71839     -0.00161961    0.51031059   -
0.00317378    0.15400499
  733   21     2.42025     8.28348    -0.58531     -0.00201125    0.51031059   -
0.00394123    0.15401395
  734   21     1.66314     8.28789    -1.64669     -0.00167116    0.51031059   -
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0.00378855    0.15500566
  739   21    -0.84631     8.29803     1.74489     -0.00173601    0.51031059   -
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  742    9     2.30365     7.95657     1.45240     -0.00162576    0.50558103   -
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0.00325236    0.15056468
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0.00294430    0.14463689
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0.00198347    0.15652487
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0.00339480    0.15149899
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  751   15     0.41186    -7.01743    -1.79561      0.00005436    0.08528603
0.00063734    0.14292589
  752   10    -0.63741    -6.16805    -2.19558     -0.00010370    0.08528603   -
0.00121590    0.15316053
  753   18    -2.98743    -1.82990    -3.75215     -0.00154432    0.75802513   -
0.00203730    0.16851607
  754   18    -3.55440    -2.80170    -3.65163     -0.00425001    1.51652287   -
0.00280247    0.16738114
  755   18    -4.14291    -3.74926    -2.84101     -0.00407413    1.51652287   -
0.00268650    0.16401271
  756   18    -4.40297    -4.10909    -1.80233     -0.00128392    0.75802513   -
0.00169377    0.15908729
  757   10    -2.09714    -2.84372    -3.68722     -0.00443990    1.51652287   -
0.00292768    0.17315033
  758   10    -2.77232    -3.97646    -3.28431     -0.00458948    1.51652287   -
0.00302632    0.16921346
  759   10    -3.20975    -4.63516    -2.15467     -0.00416990    1.51652287   -
0.00274964    0.16663264
  760   17    -4.17438    -4.18784     2.00063     -0.00134734    0.75370927   -
0.00178761    0.15943162
  761   17    -3.99363    -3.75385     2.97977     -0.00385631    1.50735899   -
0.00255832    0.16327114
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  763   17    -3.03142    -1.79985     3.81592     -0.00143547    0.75370927   -
0.00190453    0.16713795
  764   11    -2.92944    -4.64975     2.43471     -0.00345507    1.50735899   -
0.00229213    0.16512379
  765   11    -2.60036    -3.91857     3.49351     -0.00412972    1.50735899   -
0.00273970    0.16767080
  766   11    -2.03225    -2.77526     3.85966     -0.00418892    1.50735899   -
0.00277898    0.17183747
  767   14     5.63733    -1.97382    -2.54276     -0.00126619    0.76453195   -
0.00165617    0.15426977
  768   14     6.04844    -2.36608    -1.89799     -0.00090982    0.76453195   -
0.00119003    0.15106531
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  771   16     5.84931    -2.24603     2.19413     -0.00306768    1.42734123   -
0.00214923    0.15785974
  772   12     6.21089    -1.27265     1.21730     -0.00470180    1.42734123   -
0.00329410    0.16897741
  773   12     5.67525    -0.93710     2.09746     -0.00161304    0.71350655   -
0.00226072    0.16709907
  774   19    -6.40151     3.07396     1.65328     -0.00132891    0.76301858   -
0.00174164    0.15217494
  775   19    -6.87190     3.34544     0.70563     -0.00376560    1.52594894   -
0.00246771    0.15495527
  776   19    -6.87321     3.32525    -0.62934     -0.00370501    1.52594894   -
0.00242800    0.15489300
  777   19    -6.40468     3.02523    -1.56927     -0.00123907    0.76301858   -
0.00162391    0.15216375
  778   13    -5.90230     4.33746     1.28758     -0.00403387    1.52594894   -
0.00264352    0.15790450
  779   13    -6.26729     4.53973     0.01934     -0.00434021    1.52594894   -
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D.9.3 SOLUTES

The Sigma Profile of Solutes can be accessed from https://apps.che.vt.edu/Liu-2013/VT-Databases.html