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ARTICLE



# Abraham model correlations for describing dissolution of organic solutes and inorganic gases in dimethyl carbonate

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## ABSTRACT

Experimental solubility data are reported for anthracene, biphenyl, benzil, benzoin, 1-chloroanthraquinone, phenothiazine, pyrene, salicylamide, thioxanthen-9-one, xanthene, benzoic acid, 4-*tert*-butylbenzoic acid, 4-chloro-3-nitrobenzoic acid, 3,4-dichlorobenzoic acid, 3,4-dimethoxybenzoic acid, 2-hydroxybenzoic acid, 4-methoxybenzoic acid, 2-methylbenzoic acid, 3-methylbenzoic acid, 3-methyl-4-nitrobenzoic acid, 4-nitrobenzoic acid and 3,4,5-trimethoxybenzoic acid dissolved in dimethyl carbonate at 298.15 K. Abraham model correlations are derived for solute transfer into dimethyl carbonate by combining our measured solubility data with published activity coefficient and solubility data retrieved from the published chemical and engineering literature. The derived Abraham model correlations back-calculate the 52 experimental molar solubilities and infinite dilution activity coefficients to within 0.13 log units.

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Solubilities of crystalline organic compounds; dimethyl carbonate solvent; Abraham model correlations for solute transfer properties

## 1. Introduction

Organic solvents are widely utilised in manufacturing processes as a liquid medium for the synthesis of new chemical materials, as degreasing and cleaning agents for industrial machinery, as additives in drug formations and cosmetic products, as extraction solvents for removal of unwanted impurities from synthesised chemical products, and as mobile phases for preparative chromatography. Organic solvents serve as dispersing agents in varnish and paint products, are used in recrystallisation and can be added to aqueous solutions to precipitate ionic compounds. Several million tons of hazardous, petroleum-based solvents are consumed and disposed of each year by the manufacturing sector. Solvent consumption and disposal are expected to increase in the future in order to meet the societal demands of a growing population and its strong desire for an improved quality of life. Governmental regulations regarding worker safety and waste disposal will require the manufacturing sector to phase out the more hazardous solvents with less toxic replacement solvents to diminish the negative environmental impact caused by increased solvent usage. Replacement of harmful organic solvent is not an easy task as many factors must be carefully considered in order to find a suitable replacement solvent for a specific industrial application. The published chemical literature contains an enormous amount of information regarding the physical properties of liquid organic compounds, such as boiling point temperatures, melting point

temperatures, vapour pressures, densities, heat capacities, and surface tensions. Relatively little information is available in the published chemical and engineering literature regarding health/safety issues and the solubilising properties of many of the potential solvent candidates. More information is needed in these latter two areas to assist the manufacturing sector if solvent replacement objectives are to be achieved.

For the past two decades, we have been studying the dissolution of organic solutes and inorganic gases in a wide range of different organic mono-solvents [1–11], ionic liquid solvents [12–20], binary organic solvent mixtures [21–26] and aqueous-organic solvent mixtures [27–32] in order to gain a better understanding of how molecular solute–solvent and solvent–solvent interactions affect the solubilisation processes. Our measured solubility and enthalpic data [33–36] have led to the development of Abraham solvation parameter model expressions to correlate the logarithms of a solute’s gas-to-organic solvent partition coefficients,  $\log K$ , the logarithms of a solute’s water-to-organic solvent partition coefficient,  $\log P$ , the logarithm of the solute’s molar solubility,  $\log C_{\text{solute},\text{org solv}}^{\text{sat}}$ , and the solute’s molar enthalpy of solvation,  $\Delta H_{\text{solv}}$ . Expressed in terms of partition coefficients and molar solubilities, the Abraham solvation parameter model takes the mathematical forms of:

$$\log P \text{ and } \log \left( \frac{C_{\text{solute},\text{org solv}}^{\text{sat}}}{C_{\text{solute},\text{water}}^{\text{sat}}} \right) = c_p + e_p \cdot E + s_p \cdot S + a_p \cdot A + b_p \cdot B + v_p \cdot V \quad (1)$$

$$\log K \text{ and } \log \left( \frac{C_{\text{solute},\text{org solv}}^{\text{sat}}}{C_{\text{solute},\text{gas phase}}^{\text{sat}}} \right) = c_k + e_k \cdot E + s_k \cdot S + a_k \cdot A + b_k \cdot B + l_k \cdot L \quad (2)$$

Solute solubilities are given in terms of two molar solubility ratios,  $\left( \frac{C_{\text{solute},\text{org solv}}^{\text{sat}}}{C_{\text{solute},\text{water}}^{\text{sat}}} \right)$  and  $\left( \frac{C_{\text{solute},\text{org solv}}^{\text{sat}}}{C_{\text{solute},\text{gas phase}}^{\text{sat}}} \right)$ , where the subscripts ‘org solv’, ‘water’ and ‘gas phase’ denote the phase to which the molar solubility pertains. In other words, the quantities  $C_{\text{solute},\text{org solv}}^{\text{sat}}$  and  $C_{\text{solute},\text{water}}^{\text{sat}}$  represent the molar solubility of the solute in the organic solvent and in water, respectively. The quantity  $C_{\text{solute},\text{gas phase}}^{\text{sat}}$  is the molar concentration of the solute in the gas phase whose numerical value is often determined as part of the solute descriptor calculations.

Molecular solute–solvent interactions are described as the product of a solute property times the complimentary solvent property. Solute properties (or solute descriptors as they are often called) are denoted by the capitalised alphabetic characters on the right-hand side of Equations (1) and (2). Solute properties are defined as follows: **E** corresponds to the molar refraction of the given solute in excess of that of a linear alkane having a comparable molecular size; **S** is a combination of the electrostatic polarity and polarisability of the dissolved solute; **A** and **B** quantify the respective hydrogen-bond donating and hydrogen-bond accepting abilities of the solute; **V** refers to the solute’s McGowan molecular volume (calculated from atomic sizes and chemical bond numbers [37]); and **L** denotes the logarithm of the solute’s measured gas-to-hexadecane partition coefficient at 298.15 K. The complementary solvent properties ( $c_p$ ,  $e_p$ ,  $s_p$ ,  $a_p$ ,  $b_p$ ,  $v_p$ ,  $c_k$ ,  $e_k$ ,  $s_k$ ,  $a_k$ ,  $b_k$ , and  $l_k$ ) in Equations (1) and (2) are obtained by curve-fitting logarithms of experimental water-to-organic solvent partition/transfer coefficients,  $\log P$ , logarithms of experimental gas-to-organic solvent partition/transfer coefficients,  $\log K$ , and logarithms of molar solubility ratios, in accordance with the Abraham model. As indicated by Equations (1) and (2) partition coefficients and molar solubility ratios can often be included in the same mathematical correlation. The Abraham model is described in greater detail elsewhere [38–42].

The advantage of using the Abraham model to correlate partition coefficient and molar solubility data is that once the solvent properties have been determined the numerical values can be used to predict  $\log P$ ,  $\log \left( \frac{C_{\text{solute},\text{org solv}}^{\text{sat}}}{C_{\text{solute},\text{water}}^{\text{sat}}} \right)$ ,  $\log K$  and  $\log \left( \frac{C_{\text{solute},\text{org solv}}^{\text{sat}}}{C_{\text{solute},\text{gas phase}}^{\text{sat}}} \right)$  values for an additional 8,000 or so organic

solutes and inorganic gases in the given organic mono-solvent, ionic liquid mono-solvent, or binary solvent mixture. Solute descriptors are readily available for over 8,000 different organic, organo-metallic and inorganic compounds [43]. Solute descriptors can also be estimated from molar structure using functional and fragment group values [44,45] or from the compound's canonical smiles code [43]. Our published Abraham model correlations for approximately 120 organic mono-solvents [1–11,46–48], 90 ionic liquid mono-solvents [12–20], and for binary aqueous-methanol [49] and aqueous-ethanol [50,51] provide the manufacturing sector with a means to estimate the solubilising ability of both hazardous organic mono-solvents and potential replacement solvent candidates towards several thousand solute molecules. The fore-mentioned predictive capability is a valuable resource that can be used in the solvent selection process.

The number of organic and ionic liquid mono-solvents that we have studied thus far represent only a very small fraction of the solvents used in industrial processes. Ideally one would like to be able to calculate the solvent properties from a molecular structure in the same way that one can calculate solute descriptors. Our initial attempts at estimating solvent properties from functional group values [52,53] and based on random forest models [54] were promising given the small number of known solvent properties included in developing each predictive method. Preliminary studies further showed that experimental data-based Abraham model correlations would need to be determined for many additional organic mono-solvents in order to make significant progress in developing predictive methods for the different solvent coefficients ( $c_p$ ,  $e_p$ ,  $s_p$ ,  $a_p$ ,  $b_p$ ,  $v_p$ ,  $c_k$ ,  $e_k$ ,  $s_k$ ,  $a_k$ ,  $b_k$ , and  $l_k$ ) found in Equations (1) and (2). The solvent database used in our preliminary studies contained only a single carbonate solvent, and many of the different organic functional groups were missing. There were also very few organic solvents in the database that contained more than two functional groups. Solvents having greater chemical diversity are needed in order to properly capture the effect that molecular structure has on the solvent's polarity/polarisability and hydrogen-bonding character.

In the current study, we extend our Abraham model studies to include the dimethyl carbonate solvent. Propylene carbonate [10] and diethyl carbonate [11] are the only two alkyl carbonate solvents that we have studied thus far. Organic carbonates are an important solvent class as they exhibit low eco-toxicity and good biodegradability [55]. In fact, several published papers [56–60] have specifically referred to dimethyl carbonate as a non-toxic green solvent. Solubilities have been measured for anthracene, biphenyl, benzil, benzoin, 1-chloroanthraquinone, phenothiazine, pyrene, salicylamide, thioxanthen-9-one, xanthene, benzoic acid, 4-*tert*-butylbenzoic acid, 4-chloro-3-nitrobenzoic acid, 3,4-dichlorobenzoic acid, 3,4-dimethoxybenzoic acid, 2-hydroxybenzoic acid, 4-methoxybenzoic acid, 2-methylbenzoic acid, 3-methylbenzoic acid, 3-methyl-4-nitrobenzoic acid, 4-nitrobenzoic acid and 3,4,5-trimethoxybenzoic acid dissolved in dimethyl carbonate at 298.15 K. Results of our experimental measurements, combined with published solubility data for helium [61], neon [61], argon [61], krypton [61], xenon [61], hydrogen [61], nitrogen [61], oxygen [62], sulphur hexafluoride [61], carbon dioxide [63], tetrafluoromethane [61], hydrogen sulphide [64], methane [61], ethane [61] and ethene [61], and published infinite dilution activity coefficient data for hexane [65], heptane [66], octane [67], decane [68], cyclohexane [69], 1-hexene [70], tetrachloromethane [71], 1,2-dichloroethane [72], 1,1,1-trichloroethane [72], benzene [73], methyl *tert*-butyl ether [74], ethanol [75], 1-propanol [75] and diethyl carbonate [76] were used to derive Abraham model correlations for solute transfer into dimethyl carbonate from both water (Equation (1)) and from the gas phase (Equation (2)). In total 52 experimental data points were used in determining the solvent coefficients in each derived correlation. Addition of dimethyl carbonate to our solvent database will provide the manufacturing sector with solubilising data for one more environmentally friendly organic solvent.

## 2. Chemical materials and experimental methodology

Development of a meaningful Abraham model correlation for solute dissolution in dimethyl carbonate requires experimental partition coefficient and solubility data for a chemical diverse set of organic solutes that span as large of a range of solute descriptors as possible. In assembling the set of crystalline organic compounds for solubility determinations we selected several polycyclic aromatic hydrocarbons, several substituted benzoic acids, and several aromatic compounds having a large *S* solute descriptor. All chemicals used in the solubility measurements were purchased from commercial sources. The sample of dimethyl carbonate was dried over activated molecular sieves and distilled shortly before use. Samples of 1-chloroanthraquinone, benzil, salicylamide, xanthene, thioxanthen-9-one, pyrene, acenaphthene, and biphenyl were recrystallised three times from anhydrous methanol and dried for 3 days at a temperature of 333 K prior to use. Anthracene was recrystallised three times from anhydrous acetone and dried for 3 days in an oven at a temperature of 333 K. The carboxylic acid solutes were dried for 3 days at a temperature of 333 K prior to use. Gas chromatographic analysis (flame ionisation detector) indicated that the purities of purified samples of dimethyl carbonate, 1-chloroanthraquinone, benzil, anthracene, xanthene, biphenyl, pyrene, acenaphthene, thioxanthen-9-one and salicylamide were at least 0.997 mass fraction. Purities of the 12 carboxylic acid samples were determined by a non-aqueous titrimetric method based on the published method of Fritz and Lisicki [77]. The method was modified in that benzene was replaced by toluene for health reasons in preparing the titration solvent. Acid-base titrations with freshly standardised sodium methoxide (thymol blue indicator) indicated that the purities of benzoic acid, 4-*tert*-butylbenzoic acid, 3,4-dichlorobenzoic acid, 4-chloro-3-nitrobenzoic acid, 4-methoxybenzoic acid, 3,4-dimethoxybenzoic acid, 3,4,5-trimethoxybenzoic acid, 2-methylbenzoic acid, 3-methylbenzoic acid, 3-methyl-4-nitrobenzoic acid, 2-hydroxybenzoic acid and 4-nitrobenzoic acid were 0.998 ( $\pm 0.004$ ) mass fraction. The commercial suppliers and chemical purities of the chemicals used in the solubility measurements are summarised in Table 1.

Solubilities of the 24 crystalline organic compounds were measured using a static equilibration method followed by a spectroscopic determination of the concentration of the dissolved solute in the saturated solution based on the Beer–Lambert law. The experimental methodology that we use has been given in many of our earlier publications [61–65], and to conserve journal space will only be briefly described in this communication. Aliquots of the saturated solutions were transferred by syringe into weighed volumetric flasks after the samples had equilibrated in sealed amber glass bottles in a constant temperature water bath at  $298.15 \pm 0.05$  K for at least 3 days. The samples were periodically agitated to facilitate dissolution and mixing. The volumetric flasks containing the transferred aliquots were weighed on an electronic analytical balance. The transferred solutions were diluted quantitatively with 2-propanol. Absorbances of the diluted solutions and of the nine standard solutions of known solute concentrations were recorded on a Milton Roy Spectronic 1000 Plus spectrophotometer (Milton Roy, Rochester, NY, USA). The concentration of each diluted solution was computed from a Beer–Lambert law plot of absorbance versus concentration curve obtained from the measured absorbances of nine standard solutions of known solute molarity. The analysis wavelengths and concentration ranges used for each solute have been given in our earlier publications [78–97]. We checked to make sure that dimethyl carbonate did not absorb light at the analysis wavelengths and at the dimethyl carbonate concentrations in the diluted solutions.

Molar concentrations of the diluted samples deduced from the Beer-Law law graph were converted into mole fraction solubilities using the volume of the volumetric flasks that the solute was transferred into, the mass of the sample analysed, molar masses of the solvent and the respective solutes, and any dilutions that may have been needed in order for the sample's measured absorbance to fall on the Beer–Lambert law curve. We checked each equilibrated solid phase for possible solvate formation by determining the melting point temperature of the equilibrated solid phases recovered from the saturated solutions after the solubility measurements of each solute were completed. The melting point temperature of each equilibrated solid phase was within  $\pm 0.5$  K of

**Table 1.** Chemical sources and mass fraction purities of chemicals used in the solubility studies.

Chemical	Supplier	Purification method	Purity (Mass fraction)
Dimethyl carbonate	Acros Organics, Morris Plains, New Jersey, USA	Stored over molecular and distilled	0.997
1-Chloroanthraquinone	Aldrich Chemical Company, Milwaukee, Wisconsin, USA	Recrystallisation from anhydrous methanol	0.997
Phenothiazine	Acros Organics	Used as received	0.99
Biphenyl	Aldrich Chemical Company	Recrystallisation from anhydrous methanol	0.997
Benzil	Aldrich Chemical Company	Recrystallisation from anhydrous methanol	0.997
Anthracene	Aldrich Chemical Company	Recrystallisation from anhydrous acetone	0.997
Pyrene	Aldrich Chemical Company	Recrystallisation from anhydrous methanol	0.997
Acenaphthene	Aldrich Chemical Company	Recrystallisation from anhydrous methanol	0.997
Thioxanthen-9-one	Aldrich Chemical Company	Recrystallisation from anhydrous methanol	0.997
Salicylamide	Aldrich Chemical Company	Recrystallisation from anhydrous methanol	0.997
Benzoin	Aldrich Chemical Company	Recrystallisation from anhydrous methanol	0.997
Xanthene	Aldrich Chemical Company	Recrystallisation from anhydrous methanol	0.997
Benzoic acid	Aldrich Chemical Company	Dried for three days at a temperature of 333 K	0.998
4- <i>tert</i> -Butylbenzoic acid	TCI America Chemical Company	Dried for three days at a temperature of 333 K	0.998
4-Chloro-3-nitrobenzoic acid	Acros Organics	Dried for three days at a temperature of 333 K	0.998
3,4-Dichlorobenzoic acid	Aldrich Chemical Company	Dried for three days at a temperature of 333 K	0.998
2-Hydroxybenzoic acid	Aldrich Chemical Company	Dried for three days at a temperature of 333 K	0.997
4-Methoxybenzoic acid	Aldrich Chemical Company	Dried for three days at a temperature of 333 K	0.998
3,4-Dimethoxybenzoic acid	Acros Organics	Dried for three days at a temperature of 333 K	0.998
3,4,5-Trimethoxybenzoic acid	Aldrich Chemical Company	Dried for three days at a temperature of 333 K	0.998
2-Methylbenzoic acid	Aldrich Chemical Company	Dried for three days at a temperature of 333 K	0.998
3-Methylbenzoic acid	Aldrich Chemical Company	Dried for three days at a temperature of 333 K	0.998
3-Methyl-4-nitrobenzoic acid	Aldrich Chemical Company	Dried for three days at a temperature of 333 K	0.998
4-Nitrobenzoic acid	Acros Organics	Dried for three days at a temperature of 333 K	0.998
Toluene	Aldrich Chemical Company	None	0.998, anhydrous
Sodium methoxide, 25 mass % solution in methanol	Aldrich Chemical Company	None	
2-Propanol	Aldrich Chemical Company	None	0.99

the melting point temperature of the commercial sample or recrystallised compound prior to being in contact with the dimethyl carbonate solvent.

The experimental mole fraction and molar solubilities,  $x_{\text{solute}}^{\text{sat}}$  and  $C_{\text{solute,org solv}}^{\text{sat}}$  of the crystalline organic solutes in dimethyl carbonate are tabulated in the second column of Table 2. The numerical values represent the average of 4 to 8 independent experimental determinations, which were reproducible to within  $\pm 2.5\%$  (relative error). Mole fraction solubilities were converted to molar solubilities using Equation (3):

**Table 2.** Mole fraction and molar solubilities,  $x_{solute}^{sat}$  and  $C_{solute,org\ solv}^{sat}$  of 23 crystalline organic compounds dissolved in dimethyl carbonate at a temperature of 298.15 K.

Crystalline organic compound	$x_{solute}^{sat}$	$C_{solute,org\ solv}^{sat}$
1-Chloroanthraquinone	0.007964	0.09332
Phenothiazine	0.02441	0.2824
Biphenyl	0.2936	2.8314
Benzil	0.1314	1.3461
Anthracene	0.003139	0.03698
Pyrene	0.02394	0.2764
Acenaphthene	0.06224	0.7092
Thioxanthene-9-one	0.002529	0.02976
Salicylamide	0.04028	0.4645
Benzoil	0.01205	0.1404
Xanthene	0.07327	0.8188
Benzoic acid	0.09682	1.1179
4- <i>tert</i> -Butylbenzoic acid	0.03299	0.3767
2-Hydroxybenzoic acid	0.05483	0.6433
4-Chloro-3-nitrobenzoic acid	0.01402	0.1642
3,4-Dichlorobenzoic acid	0.004911	0.05798
4-Methoxybenzoic acid	0.006264	0.07374
3,4-Dimethoxybenzoic acid	0.004888	0.05752
3,4,5-Trimethoxybenzoic acid	0.008974	0.1051
2-Methylbenzoic acid	0.07368	0.8427
3-Methylbenzoic acid	0.07188	0.8228
3-Methyl-4-nitrobenzoic acid	0.006911	0.08126
4-Nitrobenzoic acid	0.004266	0.05029

$$C_{solute,org\ solv}^{sat} = \frac{x_{solute}^{sat}}{(1 - x_{solute}^{sat})V_{solvent} + x_{solute}^{sat}V_{solute}} \quad (3)$$

where  $V_{solvent}$  and  $V_{solute}$  represent the molar volume of dimethyl carbonate and the solutes, respectively. The numerical values used for the molar volumes of the hypothetical subcooled liquid solutes are given in our earlier publications [78–97].

To the best of our knowledge, there are no published solubility data for these organic solutes in dimethyl carbonate that we can compare our experimental values against. As an informational note, we did find an uncorrected typesetting error when comparing the mole fraction solubilities of common solutes dissolved in dimethyl carbonate versus diethyl carbonate. The mole fraction solubility of biphenyl in diethyl carbonate should be  $x_{solute}^{sat} = 0.334$ , and not  $x_{solute}^{sat} = 0.234$  as given in Table 2 of our earlier paper [11] that reported Abraham model correlations for solute dissolution in diethyl carbonate.

### 3. Results and discussion

The Abraham model often combines experimental partition coefficients and molar solubility ratios into a single mathematical correlation. In the case of crystalline and gaseous solutes, the solute transfer process is described by a molar solubility ratio. The molar solubility data given in Table 2 are converted to molar solubility ratios of  $\left(\frac{C_{solute,org\ solv}^{sat}}{C_{solute,water}^{sat}}\right)$  and  $\left(\frac{C_{solute,org\ solv}^{sat}}{C_{solute,gas\ phase}^{sat}}\right)$  by dividing  $C_{solute,org\ solv}^{sat}$  by the values of  $C_{solute,water}^{sat}$  and  $C_{solute,gas\ phase}^{sat}$  that were taken from our publications [80-87, 90-98]. Experimental solubility for 15 gaseous solutes (helium, neon, argon, krypton, xenon, hydrogen, nitrogen, oxygen, sulphur hexafluoride, carbon dioxide, tetrafluoromethane, hydrogen sulphide, methane, ethane and ethene) was reported in the published literature as either gas-to-dimethyl carbonate partition coefficients,  $K$ , or as the Henry's law constants,  $K_{Henry}$ . Henry's law constants are converted to log  $K$  values through Equation (4).

$$\log K = \log \left( \frac{RT}{K_{\text{Henry}} V_{\text{solvent}}} \right) \quad (4)$$

where  $R$  is the universal gas constant and  $T$  is the solution temperature.

In the case of the 14 liquid organic solutes (hexane, heptane, octane, decane, cyclohexane, 1-hexene, tetrachloromethane, 1,2-dichloroethane, 1,1,1-trichloroethane, benzene, methyl *tert*-butyl ether, ethanol, 1-propanol and diethyl carbonate) the published experimental data were in the form of activity coefficients determined from isothermal vapour-liquid equilibria. The published activity coefficients were extrapolated to infinite,  $\gamma_{\text{solute}}^{\infty}$ , and then converted to gas-to-dimethyl carbonate partition coefficients through standard thermodynamic relationships:

$$\log K = \log \left( \frac{RT}{\gamma_{\text{solute}}^{\infty} P_{\text{solute}}^{\circ} V_{\text{solvent}}} \right) \quad (5)$$

where  $P_{\text{solute}}^{\circ}$  is the saturated vapour pressure of a pure solute at the solution temperature, which in the present study is  $T = 298.15$  K.

The  $\log K$  values for the liquid and gaseous solutes are converted to  $\log P$  values by:

$$\log P = \log K - \log K_{\text{water}} \quad (6)$$

where  $K_{\text{water}}$  is the solute's gas-to-water partition coefficient, which is available for the different solutes considered in the current study [98–102]. We have tabulated in the eighth and ninth columns of Table 3 the numerical values of  $\log K$  and  $\log P$  values for the liquid and gases, along with the two respective solubility ratios,  $\log \left( \frac{C_{\text{solute.org solv}}^{\text{sat}}}{C_{\text{solute.gas phase}}^{\text{sat}}} \right)$  and  $\log \left( \frac{C_{\text{solute.org solv}}^{\text{sat}}}{C_{\text{solute.water}}^{\text{sat}}} \right)$ , that pertain to the crystalline organic compounds. Through our experimental solubility measurements and search of the published literature, we were able to assemble experimental data for 52 different solutes for use in developing Abraham model correlations for solute transfer into dimethyl carbonate.

There are sufficient experimental data for solutes dissolved in dimethyl carbonate for developing meaningful Abraham model correlations. Regression analysis of the experimental values in accordance with Equations (1) and (2) yielded the following two Abraham model expressions:

$$\log P \text{ and } \log \left( \frac{C_{\text{solute.org solv}}^{\text{sat}}}{C_{\text{solute.water}}^{\text{sat}}} \right) = 0.114(0.041) + 0.109(0.076)\mathbf{E} - 0.083(0.122)\mathbf{S} - 1.405(0.098)\mathbf{A} - 4.578(0.163)\mathbf{B} + 4.163(0.064)\mathbf{V} \quad (7)$$

(with  $N = 52$ ,  $SD = 0.125$ ,  $R^2 = 0.994$ ,  $F = 1611$ )

and

$$\log K \text{ and } \log \left( \frac{C_{\text{solute.org solv}}^{\text{sat}}}{C_{\text{solute.gas phase}}^{\text{sat}}} \right) = -0.616(0.065)\mathbf{E} + 1.905(0.090)\mathbf{S} + 2.123(0.096)\mathbf{A} + 0.992(0.013)\mathbf{L} \quad (8)$$

(with  $N = 52$ ,  $SD = 0.127$ ,  $R^2 = 1.000$ ,  $F = 27,296$ )

The correlations were obtained using the IBM SPSS Statistical 22 commercial software. The statistical information pertaining to each correlation is given below the respective correlation, where  $N$  refers to the number of experimental data points used in determining the equation coefficients,  $SD$  is the standard deviation,  $R^2$  corresponds to the squared correlation coefficient, and  $F$  represents the Fisher  $F$ -statistic. The standard error in each individual equation coefficient (at 95% level) is given in parenthesis after the coefficient itself. As an informational note, both the  $c_k \cdot \mathbf{C}_k$  and  $b_k \cdot \mathbf{B}$  terms were removed from Equation (8). The  $c_k$  term was removed because the calculated numerical value of the coefficient was very small ( $c_k = 0.002$ ). The  $b_k \cdot \mathbf{B}$  term was removed because



**Table 3.** Logarithms of experimental partition coefficients,  $\log P$  and  $\log K$ , logarithms of molar solubility ratios,  $\log \left( \frac{C_{\text{sat}}^{\text{solute.org.solv}}}{C_{\text{sat}}^{\text{solute.water}}} \right)$  and  $\log \left( \frac{C_{\text{sat}}^{\text{solute.org.solv}}}{C_{\text{sat}}^{\text{solute.gas.phase}}} \right)$ , and solute descriptors for organic compounds and inorganic gases dissolved in dimethyl carbonate at 298.15 K.

Solute	E	S	A	B	L	V	Log $K^a$	Log $P^b$	Ref.
Helium	0.000	0.000	0.000	0.000	-1.741	0.0680	-1.538	0.482	[61]
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	-1.438	0.522	[61]
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-0.634	0.836	[61]
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	-0.222	0.988	[61]
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	0.320	1.290	[61]
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	-1.156	0.564	[61]
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.2222	-0.844	0.956	[61]
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-0.749	0.761	[62]
Sulphur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.4643	-0.073	2.147	[61]
Tetrafluoromethane	-0.580	-0.260	0.000	0.000	-0.817	0.3203	-0.702	1.588	[61]
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	0.787	0.867	[63]
Hydrogen sulphide	0.350	0.310	0.100	0.070	0.723	0.2721	1.133	0.733	[64]
Methane	0.000	0.000	0.000	0.000	-0.323	0.2495	-0.334	1.126	[61]
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904	0.384	1.724	[61]
Ethene	0.107	0.100	0.000	0.070	0.289	0.3474	0.454	1.394	[61]
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.236	4.056	[65]
Heptane	0.000	0.000	0.000	0.000	3.130	1.0950	2.664	4.624	[66]
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	3.175	5.285	[67]
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	4.077	6.397	[68]
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	2.516	3.416	[69]
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.9110	2.368	3.528	[70]
Tetrachloromethane	0.460	0.380	0.000	0.000	2.823	0.7391	3.164	3.224	[71]
1,2-Dichloroethane	0.420	0.640	0.100	0.110	2.573	0.6352	3.477	2.207	[72]
1,1,1-Trichloroethane	0.370	0.410	0.000	0.090	2.733	0.7576	3.094	2.974	[72]
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	2.902	2.272	[73]
Methyl <i>tert</i> -butyl ether	0.024	0.220	0.000	0.590	2.380	0.8718	2.563	0.973	[74]
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	2.846	-0.824	[75]
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	3.343	-0.217	[75]
Diethyl carbonate	0.060	0.580	0.000	0.530	3.412	0.9462	4.171	1.731	[76]
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	9.171	1.6512	10.544	4.510	This work
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	8.028	4.998	This work
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242	6.732	4.782	This work
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5850	9.091	5.591	This work
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	6.750	4.390	This work
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374	9.049	4.179	This work
Xanthene	1.502	1.070	0.000	0.230	7.153	1.4152	7.623	5.123	This work
Benzoic acid	0.730	0.900	0.590	0.400	4.657	0.9317	6.738	1.598	This work
4- <i>tert</i> -Butylbenzoic acid	0.730	1.111	0.551	0.443	6.547	1.4953	8.699	3.475	This work
3,4-Dichlorobenzoic acid	0.950	0.920	0.670	0.260	5.623	1.1766	7.421	2.681	This work
4-Chloro-3-nitrobenzoic acid	1.250	1.470	0.700	0.440	6.685	1.2283	9.425	2.215	This work
4-Methoxybenzoic acid	0.899	1.250	0.620	0.520	5.741	1.1313	8.368	1.668	This work
3,4-Dimethoxybenzoic acid	0.950	1.646	0.570	0.755	6.746	1.3309	9.702	1.255	This work
3,4,5-Trimethoxybenzoic acid	1.001	1.760	0.603	0.850	7.711	1.5309	10.827	1.572	This work
2-Methylbenzoic acid	0.730	0.840	0.420	0.440	4.677	1.0726	6.286	1.986	This work
3-Methylbenzoic acid	0.730	0.890	0.600	0.400	4.819	1.0726	7.035	2.055	This work
3-Methyl-4-nitrobenzoic acid	1.040	1.336	0.525	0.500	6.266	1.2468	8.504	2.445	This work
4-Nitrobenzoic acid	0.990	1.520	0.680	0.400	5.770	1.1059	8.581	1.681	This work
Thioxanthene-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	9.082	4.014	This work
Benzoin	1.585	2.115	0.196	0.841	9.159	1.6804	11.548	2.817	This work
Salicylamide	1.160	1.650	0.630	0.480	5.910	1.0315	9.025	1.421	This work
Phenothiazine	1.890	1.560	0.310	0.300	8.389	1.4789	9.954	4.551	This work
2-Hydroxybenzoic acid	0.900	0.850	0.730	0.370	4.732	0.9904	7.078	1.718	This work

<sup>a</sup> For crystalline solutes, the tabulated value is  $\log \left( \frac{C_{\text{sat}}^{\text{solute.org.solv}}}{C_{\text{sat}}^{\text{solute.gas.phase}}} \right)$ .

<sup>b</sup> For crystalline solutes, the tabulated value is  $\log \left( \frac{C_{\text{sat}}^{\text{solute.org.solv}}}{C_{\text{sat}}^{\text{solute.water}}} \right)$ .

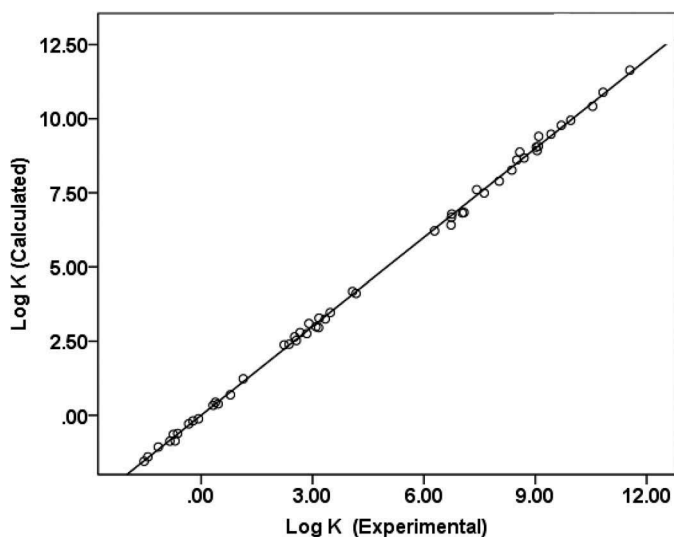


Figure 1. Comparison between the experimental  $\log K$  and  $\log \left( \frac{c_{\text{solute.org.solv}}^{\text{sat}}}{c_{\text{solute.gas.phase}}^{\text{sat}}} \right)$  data and back-calculated values based on Equation 8.

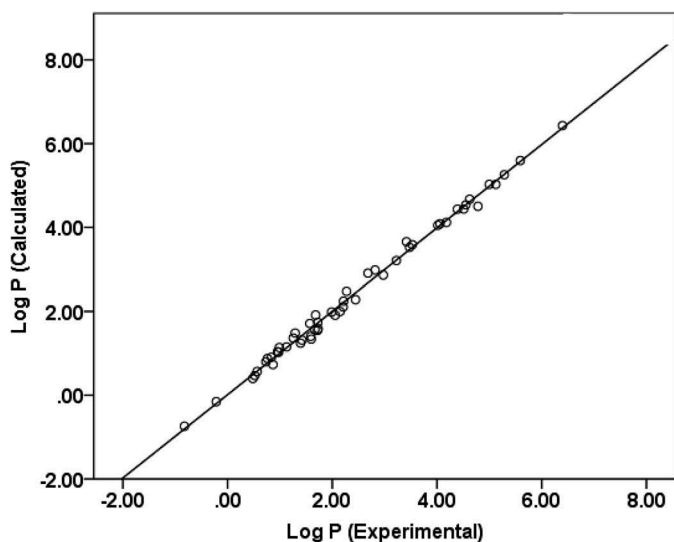


Figure 2. Comparison between the experimental  $\log P$  and  $\log \left( \frac{c_{\text{solute.org.solv}}^{\text{sat}}}{c_{\text{solute.water}}^{\text{sat}}} \right)$  data and back-calculated values based on Equation 7.

dimethyl carbonate lacks an acidic hydrogen and therefore cannot act as a hydrogen-bond donor. Removal of  $b_k \cdot \mathbf{B}$  in Equation (8) is consistent with this structural feature. As an informational note, the removal of the two terms led to an insignificant increase in the standard deviation, from  $SD = 0.121$  to  $SD = 0.127$  log units. The  $b_p \cdot \mathbf{B}$  term was retained in Equation (7), however, as the expression pertains to solute transfer into dimethyl carbonate from water. Here the  $b_p$  equation coefficient represents the difference in the acidity of dimethyl carbonate and water, which does possess two acidic hydrogens capable of engagement in hydrogen-bond formation.

Both derived Abraham model correlations provide a reasonably accurate mathematical description of the observed partition coefficients and molar solubilities of solutes dissolved in dimethyl carbonate as depicted in Figures 1 and 2. The standard deviations between the back-calculated and observed experimental values are small,  $SD = 0.125$  log units (Equation (7)) and  $SD = 0.127$  log units

(Equation (8)), and the squared correlation coefficients,  $R^2 = 0.994$  (Equation (7)) and  $R^2 = 1.000$  (Equation (8)), are near unity. The partition coefficient and solubility data do cover a large range of experimental values. For example, Equation (8) was developed based on a data set that included experimental values from  $\log K = -1.538$  for helium to  $\log K = 11.548$  for benzoin. A slightly smaller range of experimental values, from  $\log P = -0.824$  to  $\log P = 6.397$ , was used in determining the solvent coefficients given in Equation (7). The large range of experimental values covered by the solutes was made possible through the inclusion of the inorganic gases and the liquid and crystalline organic compounds in both the  $\log K$  and  $\log P$  data sets. Equations (7) and (8) are based on a firm understanding of how molecular interact in solution, and should enable journal readers to estimate partition coefficients, molar solubilities and infinite dilution activity coefficients for several thousand additional organic and inorganic solutes dissolved in dimethyl carbonate at 298 K. Partition coefficients predicted by the Abraham model can be transformed into  $\gamma_{solute}^\infty$  values through Equations (5) and (6). Solute descriptors are readily available for over 8,000 different organic, organometallic and inorganic compounds [43].

Dimethyl carbonate is the third carbonate solvent that we have studied. Previously, we determined Abraham model correlations for propylene carbonate [10]:

$$\log P \text{ and } \log \left( \frac{C_{solute,org\ solv}^{sat}}{C_{solute,water}^{sat}} \right) = 0.004 + 0.168 \mathbf{E} + 0.504 \mathbf{S} - 1.283 \mathbf{A} - 4.407 \mathbf{B} + 3.421 \mathbf{V} \quad (9)$$

$$\log K \text{ and } \log \left( \frac{C_{solute,org\ solv}^{sat}}{C_{solute,gas\ phase}^{sat}} \right) = -0.356 - 0.413 \mathbf{E} + 2.587 \mathbf{S} + 2.207 \mathbf{A} + 0.455 \mathbf{B} + 0.719 \mathbf{L} \quad (10)$$

and for diethyl carbonate [11]:

$$\log P \text{ and } \log \left( \frac{C_{solute,org\ solv}^{sat}}{C_{solute,water}^{sat}} \right) = 0.133 + 0.135 \mathbf{E} - 0.309 \mathbf{S} - 1.532 \mathbf{A} - 4.816 \mathbf{B} + 4.398 \mathbf{V} \quad (11)$$

$$\log K \text{ and } \log \left( \frac{C_{solute,org\ solv}^{sat}}{C_{solute,gas\ phase}^{sat}} \right) = 0.092 - 0.598 \mathbf{E} + 1.527 \mathbf{S} + 1.942 \mathbf{A} + 0.948 \mathbf{L} \quad (12)$$

based on our measured experimental solubilities of crystalline organic compounds dissolved in the respective carbonate solvent combined with published solubility and activity coefficient data retrieved from the chemical and engineering data. Examination of the Abraham model correlations for the three alkyl carbonate solvents reveals that dimethyl carbonate correlations are fairly similar to those of diethyl carbonate. Except for the  $s_k$  (and  $s_p$ ) equation coefficients, the equation coefficients of dimethyl carbonate and diethyl carbonate are nearly identical, at least to within the combined uncertainty in each coefficient. Dimethyl carbonate does exhibit greater dipolarity/polarisability than diethyl carbonate as evidenced by the larger  $s_k$  and  $s_p$  values. Propylene carbonate has by far the largest  $s_k$  and  $s_p$  equation coefficients, however. Propylene carbonate is the better H-bond donor as evidenced by the nonzero  $b_k$  coefficient in Equation (10). The calculated  $b_k$  coefficients for dimethyl carbonate and diethyl carbonate were small and could be set equal to zero with no loss in descriptive ability.

## 4. Summary

The Abraham solvation parameter model has been shown to provide a reasonably accurate mathematical description of the observed solubility data and partition coefficient data for 52 organic and inorganic solutes dissolved in dimethyl carbonate. The overall standard deviation between the experimental data and back-calculated values based on the Abraham model correlations developed in the present study is 0.13 log units, which is comparable in terms of descriptive ability to more than 130 different organic solvents and 70 different ionic liquid solvents that we have reported previously. Of the three alkyl carbonate solvents that we have studied thus far, propylene carbonate is found to exhibit the greatest dipolarity/polarisability and H-bond donor character.

## Disclosure statement

No potential conflict of interest was reported by the authors.

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