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Enthalpy of solvation correlations for organic solutes and gases dissolved in acetonitrile and acetone

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ABSTRACT

Data have been assembled from the published literature on the enthalpies of solvation for 74 compounds dissolved in acetonitrile and for 81 compounds dissolved in acetone. It is shown that an Abraham solvation equation can be used to correlate the experimental enthalpies of solvation in acetonitrile and acetone to within standard deviations of 2.17 and 2.72 kJ/mole, respectively. The derived correlations provide very accurate mathematical descriptions of the measured enthalpy of solvation data at 298 K, which in the case of acetonitrile span a range of about 90 kJ/mole. Mathematical correlations have also been derived for predicting the enthalpies of solvation in both solvents based on the Goss modified version of the Abraham model. Expressions based on this latter model were found to correlate the experimental enthalpies of solvation to within an overall average standard deviation of 2.52 kJ/mole for the two solvents studied.

1. Introduction

Thermodynamic properties of liquid mixtures are of interest from both practical and theoretical standpoints. Organic mixtures are often used as reaction solvent media for both industrial processes involving synthesis of pharmaceutical drug molecules, manufacture of pesticides and herbicides, and purification of reaction products through crystallization, extraction and/or chromatographic separation. The latter two processes involve solute transfer between two phases. In recent years there has been considerable interest in developing theoretical models that accurately describe solute transfer from one phase to another.

The general solvation parameter model of Abraham [1–5] is one of the more successful approaches for the analysis and prediction of free energies of partition in chemical and biological systems. The method relies on two linear free energy relationships (lfers), one for processes within condensed phases

$$\mathrm{SP} = c + e \cdot \boldsymbol{E} + s \cdot \boldsymbol{S} + a \cdot \boldsymbol{A} + b \cdot \boldsymbol{B} + v \cdot \boldsymbol{V} \tag{1}$$

and one for process involving gas-to-condensed phase transfer

$$\mathrm{SP} = c + e \cdot \boldsymbol{E} + s \cdot \boldsymbol{S} + a \cdot \boldsymbol{A} + b \cdot \boldsymbol{B} + 1 \cdot \boldsymbol{L} \tag{2}$$

The dependent variable, SP, is some property of a series of solutes in a fixed phase. The independent variables, or descriptors, are solute properties as follows: **E** and **S** refer to the excess molar refraction in units of $(\mathrm{cm}^3\,\mathrm{mol}^{-1})/10$ and dipolarity/polarizability descriptors of the solute, respectively, **A** and **B** are measures of the solute hydrogen-bond acidity and basicity, **V** is the McGowan volume in units of $(\mathrm{cm}^3\,\mathrm{mol}^{-1})/100$ and **L** is the logarithm of the gas-to-hexadecane partition coefficient at 298.15 K. The regression coefficients and constants (c, e, s, a, b, v and l) are determined by regression analyses of the experimental data for the given partition process (i.e., partition coefficients, enthalpies of solvation, etc). For any fully characterized system/process (those with calculated values for the equation coefficients) further values of SP can be estimated for solutes with known values for the solute descriptors. This is the major advantage of using Eqs. (1) and (2) to correlate solute properties having environmental, pharmaceutical and chemical importance.

Unlike other linear free energy relationships that have been proposed in recent years, the Abraham model does contain provisions for predicting how the partition coefficients vary with temperature. The temperature dependence can be included directly into the model by separating each coefficient into an enthalpic and entropic component as was recently done in describing the effect of temperature on the sorption coefficients of organic gases onto humic acid [6] and onto polyurethane foams [7]. Alternatively, the temperature variation can be accounted for by developing separate Abraham model correlations for enthalpies of solvation. In recent studies we have developed mathematical correlation equations for predicting

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the enthalpies of solvation of organic vapors and gases into water, $\Delta H_{Solv,W}$, [8]:

$$\begin{aligned}\Delta H_{Solv,W}&(\text{kJ/mole})\\&= -13.310(0.457) + 9.910(0.814)\boldsymbol{E} + 2.836(0.807)\boldsymbol{S}\\&-32.010(1.102)\boldsymbol{A} - 41.816(0.781)\boldsymbol{B} - 6.354(0.200)\boldsymbol{L}\\&(\text{with } N = 368,\ \text{S.D.} = 3.68,\\&R^2 = 0.964,\ R^2_{\text{adj}} = 0.964,\ F = 1950.5)\end{aligned} \quad (3)$$

and in hexane [9], heptane [10], hexadecane [10], cyclohexane [10], benzene [10], toluene [11], carbon tetrachloride [11], chloroform [12], methanol [13], ethanol [13], 1-butanol [13], 1-octanol [8], propylene carbonate [14], dimethyl sulfoxide [14], 1,2-dichloroethane [12], *N*,*N*-dimethylformamide [15], *tert*-butanol [15], dibutyl ether [16] and ethyl acetate [16] based on the Abraham model. In Eqs. (3) and (4) *N* corresponds to the number of solutes, *R* denotes the correlation coefficient, S.D. is the standard deviation and *F* corresponds to the Fisher *F*-statistic. The standard error in each calculated equation coefficients is given in parenthesis after the respective coefficient. The derived $\Delta H_{Solv,W}$ correlations allow one to extrapolate the predicted water-to-organic solvent partition coefficients, *P*, and gas-to-organic solvent partition coefficients, *K*, based on the Abraham model to other temperatures in the 283–328 K range. Most of the partition coefficient correlations that we have reported for water-to-organic solvents and for gas-to-organic solvents have been for 298.15 K.

The present communication represents that last of our planned enthalpy of solvation studies. We report the Abraham model correlations for enthalpies of solvation of organic vapors and gases in both acetonitrile and acetone. Predictive correlations are also derived for a second linear free energy relationship, namely the Abraham model as modified by Goss [17–21]

$$\Delta H_{Solv}(\text{kJ/mole}) = c + s\cdot\boldsymbol{S} + a\cdot\boldsymbol{A} + b\cdot\boldsymbol{B} + l\cdot\boldsymbol{L} + v\cdot\boldsymbol{V} \quad (4)$$

where the lower case letters *c*, *s*, *a*, *b*, *l* and *v* again represent the properties of the solvent. The latter model uses the five Abraham solute descriptors **S**, **A**, **B**, **V** and **L**. The Abraham **E** solute descriptor in equations such as Eqs. (2) and (3) is replaced by the Abraham **V** solute descriptor, which is easily calculable from the individual atomic sizes and number of bonds in the molecule [1,22]. More than 40 different water-to-organic solvent, gas-to-organic solvent, gas-to-humic acid, and gas-to-folvic acid partition systems have been reported in the published chemical and environmental literature based on the Abraham model as modified by Goss. In addition, we have reported modified Abraham model correlations for enthalpies of solvation of organic vapors and gases and in carbon tetrachloride [16]

$$\begin{aligned}\Delta H_{Solv,CT}&(\text{kJ/mole})\\&= -3.714(0.708) - 6.522(0.085)\boldsymbol{S} - 1.553(1.093)\boldsymbol{A}\\&-6.982(0.730)\boldsymbol{B} - 6.451(0.408)\boldsymbol{L} - 9.325(1.763)\boldsymbol{V}\\&(\text{with } N = 177,\ \text{S.D.} = 2.054,\ R^2 = 0.984)\end{aligned} \quad (5)$$

in water [16] and in the other 18 organic solvents mentioned above. While we personally prefer to use the Abraham model for the reasons discussed previously [23]; however, we do recognize that the Goss modification is now being used to correlate experimental partition coefficient and sorption coefficient data. It is only natural that the limitations and applications of this modified form of the Abraham model be further explored using ΔH_{Solv} data for solutes dissolved in acetonitrile and acetone.

There are advantages associated with having correlations based on both models, particularly in those instances where one has limited experimental data. For example, it is possible to calculate the numerical values of solute descriptors of additional compounds by combining correlations based on the Abraham model and the Goss modified Abraham model. Both models contain the Abraham solute descriptors, and by combining the derived correlations from both models one can double the number of mathematical equations that are available for solute descriptor computations. This application has been illustrated in detail elsewhere [24].

2. Data sets and solute descriptors

Our search of the chemical literature found a large number of papers [25–83] that reported experimental partial molar enthalpies of solution of liquid and crystalline organic compounds in the two solvents of interest. The latter data were determined by either direct calorimetric methods or calculated based on the temperature dependence of measured infinite dilution activity coefficient data, and the published values were converted to gas-to-organic solvent enthalpies of transfer by

$$\text{Liquid solutes}: \Delta H_{Solv} = \Delta H_{Soln} - \Delta H_{Vap,298\ \text{K}} \quad (6)$$

$$\text{Crystalline solutes}: \Delta H_{Solv} = \Delta H_{Soln} - \Delta H_{Sub,298\,\text{K}} \quad (7)$$

subtracting the solute's standard molar enthalpy of vaporization [84], $\Delta H_{Vap,298\text{K}}$, or standard molar enthalpy of sublimation [85], $\Delta H_{Sub,298\text{K}}$, at 298.15 K.

Based on an initial assessment of the available experimental data, we eliminated from consideration all experimental data that pertained to temperatures outside of the temperature range of 283–318 K. Enthalpies of solvation are temperature dependent, and we did not want to introduce large errors in the database by including experimental data far removed from 298 K. Also excluded were values based on solubility measurements where the equilibrium solid phase might be a solvated form of the solid solute. For several solutes there were multiple, independently determined values. In such cases, we selected direct calorimetric data over indirect values based on the temperature dependence of measured solubilities or infinite dilution activity coefficients. Using the forementioned criteria, 74 molar enthalpies of solvation in acetonitrile and 81 molar enthalpies of solvation in acetone were selected for regression analysis. The experimental $\Delta H_{Solv,ACN}$ and $\Delta H_{Solv,ACE}$ values are listed in Supplemental Material, Tables 1 and 2, respectively.

Molecular descriptors for all of the compounds considered in the present study are also tabulated in Supplemental Material, Tables 1 and 2. The tabulated values came from our solute descriptor database, which now contains values for more than 3500 different organic and organometallic compounds. The descriptors were obtained exactly as described before, using various types of experimental data, including water to solvent partitions, gas to solvent partitions, solubility and chromatographic data [5]. Solute descriptors used in the present study are all based on experimental data. There is also commercial software [86] and several published estimation schemes [22,87–90] available for calculating the numerical values of solute descriptors from molecular structural information if one is unable to find the necessary partition, solubility and/or chromatographic data.

3. Results and discussion

We have assembled in Supplemental Material, Table 1 values of $\Delta H_{Solv,ACN}$ for 74 organic vapors and gases dissolved in acetonitrile covering a reasonably wide range of compound type and descriptor value. Analysis of the experimental data yielded the following two

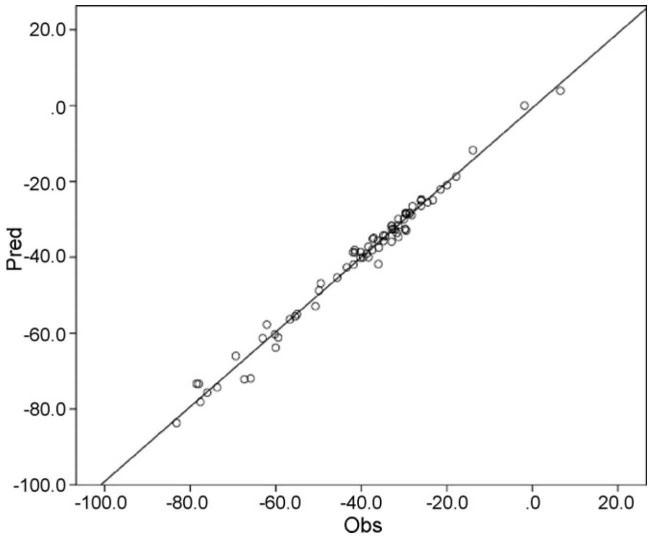

Fig. 1. A plot of the calculated values of $\Delta H_{Solv,ACN}$ (kJ/mole) based on Eq. (8) against the observed values.

Abraham model correlation equations:

$$\begin{aligned}\Delta H_{Solv,ACN}(\text{kJ/mole}) &= -4.148(0.657) + 3.304(1.215)\boldsymbol{E} - 18.430(1.239)\boldsymbol{S}\\ &\quad -26.104(1.385)\boldsymbol{A} - 7.535(1.050)\boldsymbol{B} - 6.727(0.254)\boldsymbol{L}\\ &\quad (\text{with } N = 74,\ \text{S.D.} = 2.171,\ R^2 = 0.985,\ F = 900.39)\end{aligned} \tag{8}$$

$$\begin{aligned}\Delta H_{Solv,ACN}(\text{kJ/mole}) &= 2.650(1.109) - 3.000(1.410)\boldsymbol{E}\\ &\quad -25.559(1.644)\boldsymbol{S} - 30.397(1.801)\boldsymbol{A}\\ &\quad -6.741(1.363)\boldsymbol{B} - 24.961(1.247)\boldsymbol{V}\\ &\quad (\text{with } N = 74,\ \text{S.D.} = 2.781,\ R^2 = 0.976,\ F = 543.5)\end{aligned} \tag{9}$$

All regression analyses were performed using Version 16 of the SPSS statistical software. There is little intercorrelation between the descriptors in Eqs. (8) and (9). The maximum intercorrelation is $R^2 = 0.403$ (Eq. (8)) and $R^2 = 0.582$ (Eq. (9)) between the **E** and **S** solute descriptors. The intercorrelation between the **E** and **S** solute descriptors has been noted in earlier papers [91–94]. Both Eqs. (8) and (9) provide a good statistical fit of the observed data with standard deviations of 2.171 and 2.781 kJ/mole for a data set that covers a range of 89.73 kJ/mole. See Fig. 1 for a plot of the calculated values $\Delta H_{Solv,ACN}$ based on Eq. (8) against the observed values. Eq. (8) is the better equation statistically, and from a thermodynamic standpoint Eq. (8) is the enthalpic derivative of the Abraham model's gas-to-condensed phase transfer equation. Eq. (9) might be more useful in some predictive applications in instances where the **L**-descriptor is not known. Eq. (9) uses the McGowan volume, **V**-descriptor, which is easily calculable from the individual atomic sizes and numbers of bonds in the molecule [1,22]. To our knowledge, Eqs. (8) and (9) are the first expressions that allow one to predict the enthalpy of solvation of gaseous solutes in acetonitrile.

In order to assess the predictive ability of Eq. (8) we divided the 74 data points into a training set and a test set by allowing the SPSS software to randomly select half of the experimental points. The selected data points became the training set and the compounds that were left served as the test set. Analysis of the experimental data in the training set gave

$$\begin{aligned}\Delta H_{Solv,ACN}(\text{kJ/mole}) &= -4.608(1.105) + 2.996(1.906)\boldsymbol{E}\\ &\quad -18.110(2.039)\boldsymbol{S} - 25.396(2.296)\boldsymbol{A}\\ &\quad -7.161(1.683)\boldsymbol{B} - 6.715(0.393)\boldsymbol{L}\\ &\quad (\text{with } N = 37,\ \text{S.D.} = 2.237,\ R^2 = 0.981,\ F = 325.5)\end{aligned} \tag{10}$$

There is very little difference in the equation coefficients for the full dataset and the training dataset correlations, thus showing that the training set of compounds is a representative sample of the total data set. The training set equation was then used to predict $\Delta H_{Solv,ACN}$ values for the 37 compounds in the test set. For the predicted and experimental values, we find S.D. = 2.144, AAE (average absolute error) = 1.665 and AE (average error) = 0.404 kJ/mole. There is therefore very little bias in using Eq. (10) with AE equal to 0.404 kJ/mole. The training set and test set analyses were performed two more times with similar results. Training and test validations were also performed for Eq. (10). To conserve journal space, we give only the test set results. The derived training set correlation for Eq. (10) predicted the 37 experimental $\Delta H_{Solv,ACN}$ values in the test set to within a S.D. = 3.223, AAE = 2.416 and AE = 0.640 Again, there is very little bias in the predictions using Eq. (10) with AE equal to 0.640 kJ/mole. An error/uncertainty of ±2 kJ/mole in the enthalpy of solvation results in an error of slightly less than 0.04 log units in extrapolating a log K value measured at 298.15 K to a temperature of 313.15. This level of predictive error will be sufficient for most practical chemical and engineering applications.

In Supplemental Material, Table 2 are collected values of the enthalpies of solvation of 81 gaseous solutes in acetone. Regression analyses of the experimental $\Delta H_{Solv,ACE}$ data in accordance with the Abraham model yielded:

$$\begin{aligned}\Delta H_{Solv,ACE}(\text{kJ/mole}) &= -4.965(0.568) + 4.290(1.295)\boldsymbol{E} - 17.026(1.406)\boldsymbol{S}\\ &\quad -36.672(1.748)\boldsymbol{A} - 3.794(1.184)\boldsymbol{B} - 7.307(0.226)\boldsymbol{L}\\ &\quad (\text{with } N = 81,\ \text{S.D.} = 2.715,\ R^2 = 0.986,\ F = 1073.3)\end{aligned} \tag{11}$$

$$\begin{aligned}\Delta H_{Solv,ACE}(\text{kJ/mole}) &= 3.411(1.028) - 3.436(1.697)\boldsymbol{E} - 25.312(1.969)\boldsymbol{S}\\ &\quad -39.209(2.486)\boldsymbol{A} - 4.076(1.679)\boldsymbol{B} - 27.314(1.228)\boldsymbol{V}\\ &\quad (\text{with } N = 81,\ \text{S.D.} = 3.719,\ R^2 = 0.973,\ F = 535.4)\end{aligned} \tag{12}$$

There is little intercorrelation between the descriptors in Eqs. (11) and (12). The maximum intercorrelation is $R^2 = 0.413$ (Eq. (11)) and $R^2 = 0.594$ (Eq. (12)) between the **E** and **S** solute descriptors. Both Eqs. (11) and (12) are statistically very good with standard deviations of 2.715 and 3.719 kJ/mole for a dataset that covers a range of 117.31 kJ/mole. Both equations were validated through training and test set analyses. Fig. 2 compares the calculated values of $\Delta H_{Solv,ACE}$ based on Eq. (11) against the observed data. To our knowledge there has been no previous attempt to correlate enthalpies of solvation for gaseous solutes in acetone.

As part of the current study mathematical correlations were also developed for acetonitrile based on the Goss Modified Abraham model.

$$\begin{aligned}\Delta H_{Solv,ACN}(\text{kJ/mole}) &= -2.794(1.255) - 18.737(1.657)\boldsymbol{S} - 26.884(1.555)\boldsymbol{A}\\ &\quad -8.128(1.039)\boldsymbol{B} - 5.007(0.750)\boldsymbol{L} - 5.818(3.170)\boldsymbol{V}\\ &\quad (\text{with } N = 74,\ \text{S.D.} = 2.232,\ R^2 = 0.984,\ R^2_{\text{adj}} = 0.983,\ F = 851.5)\end{aligned} \tag{13}$$

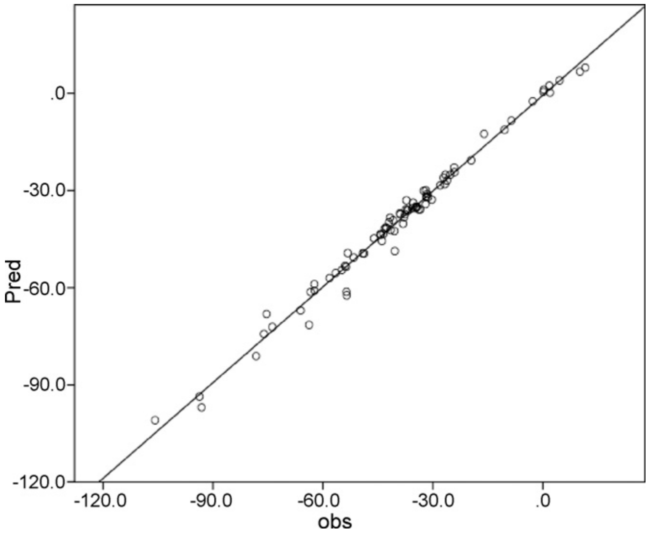

Fig. 2. A plot of the calculated values of $\Delta H_{Solv,ACE}$ (kJ/mole) based on Eq. (11) against the observed values.

and for acetone

$$\begin{aligned}
&\Delta H_{Solv,ACE}(\text{kJ/mole})\\
&\quad = -3.778(1.212) - 15.512(1.885)\boldsymbol{S} - 36.989(1.894)\boldsymbol{A}\\
&\quad -6.272(1.182)\boldsymbol{B} - 6.184(0.782)\boldsymbol{L} - 3.403(3.243)\boldsymbol{V}\\
&\quad (\text{with } N = 81,\ \text{S.D.}{=}2.820,\ R^2 = 0.984,\ R^2_{\text{adj}} = 0.983,\ F{=}942.1)
\end{aligned} \tag{14}$$

There is considerable intercorrelation between the L and V solute descriptors, $R^2 = 0.919$ (Eq. (13)) and $R^2 = 0.925$ (Eq. (14)). Strong intercorrelations between the **L** and **V** descriptors gave rise to the large standard errors that are noted in the v-coefficients.

The v · **V** term was eliminated from the model, and the experimental enthalpy of solvation data was re-analyzed to give

$$\begin{aligned}
&\Delta H_{Solv,ACN}(\text{kJ/mole})\\
&\quad = -4.784(0.642) - 16.289(1.000)\boldsymbol{S} - 25.706(1.440)\boldsymbol{A}\\
&\quad -8.961(0.951)\boldsymbol{B} - 6.326(0.216)\boldsymbol{L}\\
&\quad (\text{with } N = 74,\ \text{S.D.}{=}2.286,\ R^2 = 0.984,\ R^2_{\text{adj}}{=}0.983,\ F{=}1028.3)
\end{aligned} \tag{15}$$

and

$$\begin{aligned}
&\Delta H_{Solv,ACE}(\text{kJ/mole})\\
&\quad = -4.879(0.605) - 13.943(1.148)\boldsymbol{S} - 36.520(1.861)\boldsymbol{A}\\
&\quad -6.860(1.041)\boldsymbol{B} - 6.973(0.214)\boldsymbol{L}\\
&\quad (\text{with } N = 81,\ \text{S.D.}{=}2.841,\ R^2{=}0.984,\ R^2_{\text{adj}} = 0.983,\ F{=}1175.8)
\end{aligned} \tag{16}$$

The latter two correlations provide very good descriptions of the observed enthalpy of solvation data, and are comparable in descriptive ability to Eqs. (8) and (11) of the Abraham model. Eqs. (15) and (16) were validated through training set and test set analysis.

The correlations presented in this study further document the ability of the Abraham solvation parameter model and the Goss Modified Abraham model to describe the solute transfer properties. One can use the derived correlations based on either model to predict the ΔH_{Solv} for additional solutes dissolved in acetonitrile and in acetone. The calculated ΔH_{Solv} values can be used in conjunction with our existing correlation equations for predicting gas-to-acetonitrile and gas-to-acetone partition coefficients. Our existing correlation expressions pertain to 298.15 K. The correlations presented here allow us to extrapolate predicted log *K* values to slightly higher and lower temperatures.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.tca.2008.11.015.

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