Descriptors for Cyclooctasulfur: Estimation of Water–Solvent Partition Coefficients, Solubilities in Solvents, and Physicochemical Properties

Michael H. Abraham and William E. Acree, Jr.

1Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, U.K.
2Department of Chemistry, University of North Texas, 1155 Union Circle Drive #305070, Denton, Texas 76203-5017, United States

ABSTRACT: We have used literature data on the solubility of cyclooctasulfur in a number of solvents to drive Abraham descriptors for cyclooctasulfur. These can then be used in linear free-energy relationships that we have already constructed to predict partition coefficients and solubilities in a very large number of additional solvents. Cyclooctasulfur is very hydrophobic, has zero hydrogen bond acidity and zero hydrogen bond basicity, and dissolves best in nonpolar or only moderately polar solvents. We have also obtained enthalpies of solvation of cyclooctasulfur in solvents; again our linear free-energy relationships can be used to predict enthalpies of solvation in further solvents.

1. INTRODUCTION

The lithium/sulfur battery is a recent development. It has a high theoretical capacity, and has aroused considerable interest.1,2 One concern is the solubility of sulfur in potential nonaqueous electrolytes, and Zheng et al.3 have determined the solubility of sulfur in a several candidate solvents. However, the number of possible solvents is so large that it would be very useful to have methods of estimating the solubility of sulfur and then to use these to estimate solubilities of sulfur in other solvents method of Klamt4 to calculate the solubility of sulfur in ten solvents, but this method is very computer intensive and it would be of some advantage to have a simpler method that could be used without recourse to a specific computer software program.

We have developed a method of assigning properties or “descriptors” of molecules, based on linear free-energy relationships, LFERs. These descriptors, together with equations for water–solvent partition coefficients, that we have concurrently developed, can then be used to estimate further water–solvent partition coefficients into a very large number of solvents. Because water–solvent partition coefficients can, for the most part, be regarded as the ratio of solubilities in a solvent and in water, this provides an arithmetically very simple way of estimating solubilities. Our aim is therefore to obtain descriptors for sulfur and then to use these to estimate solubilities of sulfur in a wide range of solvents.

The stable form of solid sulfur at 298 K is orthorhombic α-sulfur5 and so any solubility at 298 K will be that of α-sulfur. There are a number of configurations of sulfur that can exist in solution. However, α-sulfur dissolves as cyclooctasulfur6 and so all of the data on solubilities that we shall use refer to cyclooctasulfur of molecular weight 256.52. Some literature data on solubilities are given in terms of cyclooctasulfur, but other data may be in terms of wt %, etc. Where necessary, we have converted solubilities given in various units to mol cyclooctasulfur per dm$^3$ solution.

2. METHODOLOGY

The method we use makes use of two LFERs, eqs 1 and 2. In eq 1, SP is $P_w$, the water—solvent partition coefficient, and in eq 2, SP is $K_w$, the dimensionless gas to solvent partition coefficient.

\[
\log SP = c + cE + sS + aA + bB + vV
\]  

(1)

\[
\log SP = c + cE + sS + aA + bB + lL
\]  

(2)

The independent variables, or descriptors, in eqs 1 and 2, are properties of a neutral solute, in this case cyclooctasulfur, as follows:7−12 E is the solute excess molar refraction in cm$^3$ mol$^{-1}$/10, S is the solute dipolarity/polarizability, A is the overall solute hydrogen bond acidity, B is the overall solute hydrogen bond basicity, V is McGowan’s characteristic molecular volume in cm$^3$ mol$^{-1}$/100,12 and L is the logarithm of the gas to hexadecane partition coefficient at 298 K. The coefficients in eqs 1 and 2 are shown in Table 1 for partition from water or from the gas phase to the various solvents that we shall deal with.13−22 These are all dry solvents except for octan-1-ol where the solvent is in equilibrium with water. We list this solvent as “wet” octan-1-ol.
Table 1. Coefficients in the LFER Equations, eqs 1 and 2

| Solvent, eq 1 | \(c\) | \(c^*\) | \(s\) | \(a\) | \(b\) | \(v\) |
|---------------|--------|--------|--------|------|------|------|
| octan-1-ol, wet | 0.088  | 0.562  | −1.054 | 0.034 | −3.460 | 3.814 |
| hexane        | 0.333  | 0.560  | −1.710 | −3.578 | −4.939 | 4.463 |
| heptane       | 0.297  | 0.634  | −1.755 | −3.571 | −4.946 | 4.488 |
| cyclohexane   | 0.159  | 0.784  | −1.678 | −3.740 | −4.929 | 4.577 |
| trichloromethane | 0.191 | 0.105  | −0.403 | −3.112 | −3.514 | 4.395 |
| tetrachloromethane | 0.199 | 0.523  | −1.159 | −3.560 | −4.594 | 4.618 |
| 1,2-dichloroethane | 0.183 | 0.294  | −0.134 | −2.801 | −4.291 | 4.180 |
| diethyl ether | 0.350  | 0.358  | −0.820 | −0.588 | −4.956 | 4.350 |
| propanone     | 0.313  | 0.312  | −0.121 | −0.608 | −4.753 | 3.942 |
| acetonitrile  | 0.413  | 0.077  | 0.326  | −1.566 | −4.391 | 3.364 |
| dimethylsulfoxide | −0.194 | 0.327  | 0.791  | 1.260  | −4.540 | 3.361 |
| dimethylformamide | −0.305 | −0.058 | 0.343  | 0.358  | −4.865 | 4.486 |
| propylene carbonate | 0.004 | 0.168  | 0.504  | −1.283 | −4.407 | 3.421 |
| aniline       | −0.156 | 0.325  | −0.006 | −1.289 | −3.512 | 3.841 |
| pyridine      | −0.056 | 0.271  | 0.082  | 0.657  | −4.638 | 4.297 |
| ethanol       | 0.222  | 0.471  | −1.035 | 0.326  | −3.596 | 3.857 |
| diethylene glycol | −0.096 | 0.58   | −0.145 | 0.138  | −3.718 | 3.072 |
| benzene       | 0.142  | 0.464  | −0.588 | −3.099 | −4.625 | 4.491 |
| toluene       | 0.125  | 0.431  | −0.644 | −3.002 | −4.748 | 4.524 |
| m-xylene      | 0.122  | 0.377  | −0.603 | −2.981 | −4.961 | 4.535 |
| ethylbenzene  | 0.093  | 0.467  | −0.723 | −3.001 | −4.844 | 4.514 |
| chlorobenzene | 0.065  | 0.381  | −0.521 | −3.183 | −4.700 | 4.614 |
| nitrobenzene  | −0.152 | 0.525  | 0.081  | −2.332 | −4.494 | 4.187 |
| carbon disulfide | 0.047 | 0.686  | −0.943 | −3.603 | −5.818 | 4.921 |
| gas to water, log \(K_a\) | −0.994 | 0.577  | 2.549  | 3.813  | 4.841 | −0.869 |

| Solvent, eq 2 | \(c\) | \(c^*\) | \(s\) | \(a\) | \(b\) | \(j\) |
|---------------|--------|--------|--------|------|------|------|
| octan-1-ol, wet | −0.222 | 0.088  | 0.701  | 3.473 | 1.477 | 0.851 |
| hexane        | 0.320  | 0.000  | 0.000  | 0.000 | 0.000 | 0.945 |
| heptane       | 0.284  | 0.000  | 0.000  | 0.000 | 0.000 | 0.950 |
| cyclohexane   | 0.163  | −0.110 | 0.000  | 0.000 | 0.000 | 1.013 |
| trichloromethane | 0.157 | −0.560 | 1.259  | 0.374 | 1.333 | 0.976 |
| tetrachloromethane | 0.217 | −0.435 | 0.554  | 0.000 | 0.000 | 1.069 |
| 1,2-dichloroethane | 0.017 | −0.337 | 1.600  | 0.774 | 0.637 | 0.921 |
| diethyl ether | 0.288  | −0.379 | 0.904  | 2.937 | 0.000 | 0.963 |
| propanone     | 0.217  | −0.387 | 1.733  | 3.060 | 0.000 | 0.866 |
| acetonitrile  | −0.007 | −0.595 | 2.461  | 2.085 | 0.418 | 0.738 |
| dimethylsulfoxide | −0.556 | −0.223 | 2.903  | 5.037 | 0.000 | 0.719 |
| dimethylformamide | −0.391 | −0.869 | 2.107  | 3.774 | 0.000 | 1.011 |
| propylene carbonate | −0.356 | −0.413 | 2.587  | 2.207 | 0.455 | 0.719 |
| aniline       | −0.394 | −0.362 | 1.895  | 2.421 | 1.334 | 0.842 |
| pyridine      | −0.145 | −0.416 | 1.915  | 4.443 | 0.000 | 0.946 |
| ethanol       | 0.017  | −0.232 | 0.867  | 3.894 | 1.192 | 0.846 |
| diethylene glycol | −0.496 | 0.167  | 1.961  | 3.831 | 1.057 | 0.617 |
| benzene       | 0.107  | −0.313 | 1.053  | 0.457 | 0.169 | 1.020 |
| toluene       | 0.085  | −0.400 | 1.063  | 0.501 | 0.154 | 1.011 |
| m-xylene      | 0.071  | −0.423 | 1.068  | 0.522 | 0.000 | 1.014 |
| ethylbenzene  | 0.059  | −0.295 | 0.924  | 0.573 | 0.098 | 1.030 |
| chlorobenzene | 0.064  | −0.399 | 1.151  | 0.313 | 0.171 | 1.032 |
| nitrobenzene  | −0.296 | 0.092  | 1.707  | 1.147 | 0.443 | 0.912 |
| carbon disulfide | 0.101 | 0.251  | 0.177  | 0.027 | 0.095 | 1.068 |
| gas to water, log \(K_a\) | −1.271 | 0.822  | 2.743  | 3.904 | 4.814 | −0.213 |

Use of eqs 1 and 2 for the determination of descriptors has been reviewed several times.7−11 In brief, a set of simultaneous equations is set up using eqs 1 and 2 with known values of the dependent variable for a given compound. The values of the independent variables, \(E, S, A, B, V\), and \(L\), are then obtained by using solution of the set of simultaneous equations. Because we invariably have more equations than unknowns, the set of equations is solved by trial-and-error, with the final set of independent variables, or descriptors, taken as the set that yields the smallest error of the fit. The “Solver” add-on to the Microsoft Excel is a particularly convenient method to obtain the trial-and-error solution.

3. RESULTS AND DISCUSSION

The solubility data that we use are given in Table 2 as log \(C_s\) where \(C_s\) is the solubility of \(S_8\) in mol dm\(^{-3}\). These solubilities
can be transformed into water—solvent partition coefficients through eq 3, where \( C_w \) is the solubility of \( S_8 \) in water at 298 K.

### Table 2. Solubilities of Cyclooctasulfur in Solvents at 298 K

| solvent                  | solubility as \( \log(\text{mol} \ S_8 \text{ dm}^{-3}) \) |
|--------------------------|----------------------------------------------------------|
| trichloromethane         | -1.290,29 -1.17329                                       |
| tetrachloromethane       | -1.513,23 -1.285,24 -1.275,26                           |
| 1,2-dichloroethane       | -1.397,29                                               |
| benzene                  | -1.101,23 -1.146,23 -1.099,23                           |
| toluene                  | -1.107,23 -1.196,27 -1.136,30                           |
| m-xylene                 | -1.180,29                                               |
| ethylbenzene             | -1.483,30                                               |
| chlorobenzene            | -0.993,30 -0.873,30                                      |
| nitrobenzene             | -1.392,29                                               |
| diethyl ether            | -1.923,33 -2.107,29                                      |
| carbon disulfide         | 0.243,26                                                |
| ethanol                  | -2.695,6 -2.768,3                                        |
| propanone                | -1.085,6 -2.616,29 -2.676,3                             |
| hexane                   | -2.113,4 -2.150,4 -2.593,5                              |
| heptane                  | -2.018,13                                               |
| cyclohexane              | -1.471,28 -1.271,13                                      |
| acetonitrile             | -3.214,4                                                |
| pyridine                 | -1.318,3                                                |
| dimethylformamide        | -2.297,1                                                |
| aniline                  | -1.300,29                                               |
| propylene carbonate      | -2.880,1                                                |
| dimethylsulfide          | -2.404,1                                                |
| \( \gamma \)-butyrolactone | -2.410,1                                        |
| dimethoxyethane          | -2.002,2                                                |
| diglyme                  | -1.989,3 -2.155,25                                       |
| triglyme                 | -2.137,25                                               |
| tetraglyme               | -2.128,25                                               |
| diethyleneglycol         | -2.958,15                                               |
| cyclohexene              | -1.081,20                                               |
| 1,2,3,4-tetrahydro-naphthalene | -1.066,20                                    |
| styrene                  | -1.175,30                                               |

### Table 3. Calculation of the Enthalpy of Solvation of Cyclooctasulfur in kJ mol\(^{-1}\) at 298 K

| solvent                  | \( \Delta H_{\text{sublimation}} \) | \( \Delta H_{\text{solution}} \) | \( \Delta H_{\text{solv}} \) |
|--------------------------|--------------------------------------|------------------------------------|-----------------------------|
| benzene                  | 100.1                                | 25.2                               | -74.9                       |
| toluene                  | 100.1                                | 25.1                               | -75.0                       |
| ethylbenzene             | 100.1                                | 30.1                               | -70.0                       |
| tetrail                  | 100.1                                | 22.9                               | -77.2                       |
| styrene                  | 100.1                                | 44.0                               | -56.1                       |
| chlorobenzene            | 100.1                                | 22.9                               | -77.2                       |
| hexane                   | 100.1                                | 53.3                               | -46.8                       |
| cyclohexane              | 100.1                                | 23.0                               | -77.1                       |

### Table 4. Equations for the Calculation of Enthalpy of Solvation into Various Solvents

| Solvent, eq in V | \( c \) | \( e \) | \( s \) | \( a \) | \( b \) | \( y \) |
|------------------|--------|--------|--------|--------|--------|--------|
| benzene          | 3.396  | -4.108 | -20.296| -12.198| -4.174 | -31.095|
| toluene          | 4.199  | -7.143 | -20.440| -10.006| -3.439 | -32.235|
| chlorobenzene    | 5.534  | -4.164 | -20.543| -16.252| -4.832 | -34.675|
| hexane           | 4.894  | -8.916 | -8.463 | -1.168 | 0.773  | -36.769|

### Table 5. Values of \( P_{\text{oct}} \), a Measure of Hydrophobicity

| solute                        | \( \log P_{\text{oct}} \) |
|-------------------------------|---------------------------|
| cyclooctasulfur               | 5.29                      |
| biphenyl                      | 4.01                      |
| cyclooctane                   | 4.45                      |
| decahydrogenaphthalene        | 4.79                      |
| octane                        | 5.18                      |
| triphenylmethane              | 5.65                      |
| decane                        | 5.98                      |

can be transformed into water—solvent partition coefficients through eq 3, where \( C_w \) is the solubility of \( S_8 \) in water at 298 K.
The observed solubility in acetonitrile seems quite out-of-line in comparison with solubilities in other polar aprotic solvents and can be classed as extremely hydrophobic. It can be seen that cyclooctasulfur is not very polar and has neither hydrogen bond acidity nor hydrogen bond basicity. The latter observation may appear surprising, but sulfur compounds in general have a low dipolarity. Other hydrophobic solutes can be classed as extremely hydrophobic.

Our obtained descriptors can now be used to calculate values of log $P_e$ for other solutes, as long as $K_w$ is not very different from that obtained from solubilities in other solvents. The latter observation is consistent with the fact that cyclooctasulfur is not a very polar compound and does not possess any hydrogen bond acceptor or donor sites. Therefore, we can expect that for other solutes, the calculated values of log $P_e$ will be similar to the observed solubilities in the solvents used for the determination of $K_w$.

We have fitted the data of Table 3 to the Apelblat equation, eq 6, and find that the values of $K_w$ are very similar to those obtained from solubilities in other solvents. The calculated solubilities are in Table 2. There are some differences between the calculated and observed solubilities, but these are generally small and within the limits of experimental error. The calculated solubilities are in Table 2.

We have used the values of $K_w$ to calculate the enthalpy of solution at 298 K and the enthalpy of solvation of each solute. These values are shown in Table 3. The enthalpies of solution were calculated from the increase in temperature, and the enthalpies of solvation were calculated from the decrease in temperature. The values are given in Table 3.

We have used these values to calculate the enthalpy of sublimation, these yield the enthalpy of solvation of cyclooctasulfur. The values are shown in Table 3.

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solubilities in a very large number of solvents, for which we have equation on the line of eq 1. As expected from the hydrophobicity of cyclooctasulfur, it is not very soluble in alcohols or in dipolar aprotic solvents but is more soluble in aliphatic or aromatic hydrocarbons. Other solvents, in which cyclooctasulfur is more soluble, are aliphatic esters and aliphatic ethers, especially cyclic ethers, and a number of other not very polar solvents, such as cyclohexanone and N-methylpyrrolidinone, see Table 6. We also have equations for enthalpy of solvation in additional solvents to those in Table 4, and so enthalpies of solvation can be predicted for these extra solvents.

Because of its high hydrophobicity it seemed unlikely that cyclooctasulfur would easily be soluble in solvents, such as ionic liquids. We have equations for partition into a large number of ionic liquids. We have equations for partition into a large number of ionic liquids, solubilities are very low, even lower that in the dipolar aprotic liquids, listed in Table 2. This example shows again how simple it is to estimate solubilities for cyclooctasulfur using the equations that we have assembled.

**AUTHOR INFORMATION**

**Corresponding Author**

*E-mail: m.h.abraham@ucl.ac.uk.*

**ORCID**

Michael H. Abraham: 0000-0002-4579-8621

William E. Acree Jr.: 0000-0002-1177-7419

**Notes**

The authors declare no competing financial interest.

**REFERENCES**

(1) Barchasz, C.; Molton, F.; Duboc, C.; Lepretre, J.-C.; Patoux, S.; Alloin, F. Lithium/sulfur cell discharge mechanism: an original approach for intermediate species identification. *Anal. Chem.* 2012, 84, 3973–3980.

(2) Borghamadi, M.; Best, A. S.; Bhatt, A. I.; Hollenkamp, A. F.; Musameh, M.; Rees, R. J.; Ruther, T. Lithium-sulfur batteries – the solution is in the electrolyte but is the electrolyte a solution? *Energy Environ. Sci.* 2014, 7, 3902–3920.

(3) Zheng, D.; Zhang, X.; Li, C.; McKinnon, M. E.; Sadok, R. G.; Qu, D.; Yu, X.; Lee, H.-S.; Yang, X.-Q.; Qu, D. Quantitative chromatographic determination of dissolved elemental sulfur in the non-aqueous electrolyte for lithium-sulfur batteries. *J. Electrochem. Soc.* 2015, 162, A203–A206.

(4) Jeschke, S.; Johansson, P. Predicting the solubility of sulfur: a COSMO-RS-based approach to investigate electrolytes for Li-S batteries. *Chem. - Eur. J.* 2017, 23, 9130–9136.

(5) Klamt, A. Conductor-like screening model for real solvents: a new approach to the quantitative calculation of solvation phenomena. *J. Phys. Chem. B* 1995, 99, 2224–2235.

(6) Meyer, B. Elemental sulfur. *Chem. Rev.* 1976, 76, 367–388.

(7) Abraham, M. H. Scales of hydrogen bonding: their construction and application to physicochemical and biochemical processes. *Chem. Soc. Rev.* 1993, 22, 73–83.

(8) Abraham, M. H.; Ibrahim, A.; Zissimos, A. M. The determination of sets of solute descriptors from chromatographic measurements. *J. Chromatogr.* A 2004, 1037, 29–47.

(9) Poole, C. F.; Atapattu, S. N.; Poole, S. K.; Bell, A. K. Determination of solute descriptors by chromatographic methods. *Anal. Chem. Acta* 2009, 652, 32–53.

(10) Poole, C. F.; Ariyasena, T. C.; Lenca, N. Estimation of the environmental properties of compounds from chromatographic measurements and the solvation parameter model. *J. Chromatogr. A* 2013, 1317, 85–104.

(11) Clarke, E. D.; Mallon, L. The Determination of Abraham descriptors and their Application to Crop Protection Research. In *Modern Methods in Crop Protection Research*; Jeschke, P., Krämer, W., Schirmer, U., Witschel, M., Eds.; Wiley-VCH Verlag GmbH & Co, 2012.

(12) Abraham, M. H.; McGowan, J. C. The use of characteristic volumes to measure cavity terms in reversed-phase liquid chromatography. *Chromatographia* 1987, 23, 243–246.

(13) Abraham, M. H.; Acree, W. E., Jr.; Leo, A. J.; Hoekman, D. The partition of compounds from water and from air into wet and dry ketones. *New J. Chem.* 2009, 33, 568–573.

(14) Grubbs, L. M.; Saifullah, M.; De La Rosa, N. E.; Achi, S. S.; Acree, W. E., Jr.; Abraham, M. H. Mathematical correlations for describing solute transfer into functionalized alkane solvents containing hydroxyl, ether, ester or ketone solvents. *Fluid Phase Equilib.* 2010, 298, 48–53.

(15) Abraham, M. H.; Acree, W. E., Jr. The transfer of neutral molecules, ions and ionic species from water to ethylene glycol and to propylene carbonate; descriptors for pyridinium cations. *New J. Chem.* 2010, 34, 2298–2305.

(16) Abraham, M. H.; Andonian-Hafvan, J.; Whiting, G. S.; Leo, A.; Taft, R. W. Hydrogen bonding. Part 34: the factors that influence the solubility of gases and vapours in water at 298 K, and a new method for its determination. *J. Chem. Soc., Perkin Trans. 2* 1994, 1777–1791.

(17) Abraham, M. H.; Nasezadeh, A.; Acree, W. E., Jr. Correlation and prediction of partition coefficients from the gas phase and from water to alkane-1-ols. *Ind. Eng. Chem. Res.* 2008, 47, 3990–3905.

(18) Saifullah, M.; Ye, S.; Grubbs, L. M.; De La Rosa, N. E.; Acree, W. E., Jr.; Abraham, M. H. Abraham model correlations for the transfer of neutral molecules to tetrahydrofuran and to 1,4-dioxane and for transfer of ions to tetrahydrofuran. *J. Solution Chem.* 2011, 40, 2082–2094.

(19) Springer, L. M.; Achi, S. S.; Pointer, R.; Blake-Taylor, B. H.; Acree, W. E., Jr.; Abraham, M. H. Development of Abraham model correlation for solvation characteristics of linear alcohols. *Fluid Phase Equilib.* 2009, 286, 170–174.

(20) Springer, L. M.; Achi, S. S.; Acree, W. E., Jr.; Abraham, M. H.; Leo, A. J.; Hoekman, D. Correlation and prediction of solute transfer to chloroalkanes from both water and the gas phase. *Fluid Phase Equilib.* 2009, 281, 144–162.

(21) Abraham, M. H.; Zad, M.; Acree, W. E., Jr. The transfer of neutral molecules from water and from the gas phase to solvents acetonaphone and aniline. *J. Mol. Liq.* 2015, 212, 301–306.

(22) Abraham, M. H.; Chadha, H. S.; Whiting, G. S.; Mitchell, R. C. Hydrogen bonding. 32. An analysis of water-octanol and water-alkane partitioning, and the ΔlogP parameter of Seiler. *J. Pharm. Sci.* 1993, 84, 1085–1100.

(23) Delaplace, R. Solubility of sulfur in some organic liquids. *J. Pharm. Chem.* 1922, 26, 139–140.

(24) Jakowkin, A. A.; Archangelsky, P. A. The mutual solubility of iodine and sulfur in carbon tetrachloride. *Z. Anorg. Allg. Chem.* 1936, 226, 350–352.

(25) Sciamana, S. F.; Lynn, S. Sulfur solubility in pure and mixed organic solvents. *Ind. Eng. Chem. Res.* 1988, 27, 485–491.

(26) Austin, J. M.; Jensen, D.; Meyer, B. Solubility of sulfur in liquid sulfur dioxide, carbon disulfide and carbon tetrachloride. *J. Chem. Eng. Data* 1971, 16, 364–366.

(27) Jay, S.; Cezac, P.; Serin, J.-P.; Contamine, F.; Martín, C.; Merckadier, J. Solubility of elemental sulfur in toluene between (267.15 and 313.15) K under atmospheric pressure. *J. Chem. Eng. Data* 2009, 54, 3238–3241.

(28) Brooke, M. Solubility of sulfur: an undergraduate project. *J. Chem. Educ.* 1951, 28, 434–435.

(29) Bamberg, M. *Gmelin Handbuch der Anorganischen Chemie, Schwefel, Teil A, Lieferung 3*; VCH: Weinheim, 1953.

(30) Wang, R.; Shen, B.; Sun, H.; Zhao, J. Measurement and correlation of the solubilities of S8 in 10 solvents. *J. Chem. Eng. Data* 2018, 63, 553–558.
(31) Kamyshny, A., Jr. Solubility of cyclooctasulfur in pure water and sea water at different temperatures. *Geochim. Cosmochim. Acta* 2009, 73, 6022–6028.

(32) Boulegue, J. Solubility of elemental sulfur in water at 298 K. *Phosphorus Sulfur Relat. Elem.* 1978, 5, 127–128.

(33) Briske, C.; Hartshorne, N. H.; Stranks, D. R. The vapour pressures and latent heat of sublimation of α-, β- and γ-sulfur. *J. Chem. Soc.* 1960, 1200–1209.

(34) Varfolomeev, M. A.; Rakipov, I. T.; Khacchaturian, A. A.; Acree, W. E., Jr.; Brumfeld, M.; Abraham, M. H. Effect of halogen substitution on the enthalpies of solvation and hydrogen bonding in chlorobenzene and 1,2-dichlorobenzene derived using multi-parameter correlations. *Thermochim. Acta* 2015, 617, 8–20.

(35) Lu, J. Z.; Acree, W. E., Jr.; Abraham, M. H. Updated Abraham model correlations for enthalpies of solvation of organic solutes dissolved in benzene and acetonitrile. *Phys. Chem. Liq.* 2018, 1–16.

(36) Mintza, C.; Clark, M.; Burton, K.; Acree, W. E., Jr.; Abraham, M. H. Enthalpy of solvation correlations for gaseous solutes dissolved in toluene and carbon tetrachloride based on the Abraham model. *J. Solution Chem.* 2007, 36, 947–966.

(37) Mintza, C.; Burton, K.; Acree, W. E., Jr.; Abraham, M. H. Enthalpy of solvation correlations for gaseous solutes dissolved in linear alkanes (C5–C16) based on the Abraham model. *QSAR Comb. Sci.* 2008, 27, 179–186.

(38) BioLoom, BioByte Corp, 201 W. 4th Street, #204 Claremont, CA 91711–4707, USA.

(39) Jiang, B.; Horton, M. Y.; Acree, W. E., Jr.; Abraham, M. H. Ion-specific equation coefficient version of the Abraham model for ionic liquid solvents; determination of coefficients for tributylethylphosphonium, 1-butyl-1-methylmorpholinium, 1-allyl-3-methylimidazolium and octyltriethylammonium cations. *Phys. Chem. Liq.* 2017, 55, 358–385.