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Solubilities of Oxygenated Aromatic Solids in Pressurized Hot Water[†]

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Aqueous solubilities of xanthene ($C_{13}H_{10}O$), anthrone ($C_{14}H_{10}O$), xanthone ($C_{13}H_8O_2$), thioxanthone ($C_{13}H_8OS$), 9,10-anthraquinone ($C_{14}H_8O_2$), and 9,10-phenanthrenequinone ($C_{14}H_8O_2$) were measured at temperatures from 313 K to the solute melting point and pressures close to 5 MPa by a dynamic method combined with gas chromatography/mass spectrometry. The experimental solubilities were used to estimate the activity coefficients of the solutes in the aqueous solutions at saturation. Relative rates of increase of solute solubility (mole fraction) with temperature ranged from 0.049 K^{-1} to 0.056 K^{-1}.

Introduction

Water, the greenest of solvents, is also the most tunable single-component solvent as regards the attainable variations in relative permittivity, cohesive energy density, and ionic product that can result from changes in the operating temperature and pressure. Consequently, the solvent properties of supercritical water differ substantially from those of water at 298 K and 0.1 MPa.[1−6] Even at relatively mild conditions in pressurized hot water (= liquid water at temperatures between the normal boiling point and the critical point, PHW), a strong increase in solubilities of polycyclic aromatic hydrocarbons (PAHs) with rising temperature is apparent. Naphthalene and water become completely miscible in the liquid state above 583 K,[1] and even three- and four-ring PAHs may become miscible with PHW at certain conditions.[5] The fortunate combination of greenness and tunability gives water a specific position among the solvents and/or reaction media for sustainable processes.[7,8]

Measurements of solubilities of organic nonelectrolyte solids in PHW have largely been focused on PAHs.[9−15] To extend the available information on the solvent properties of PHW, the aqueous solubilities of a number of solid heterocycles[16] and lower diamondoids[17] were recently measured in the temperature interval between 313 K and the solute melting point. We also employed the solubility data to develop simple correlations of aqueous solubilities of the solutes within a wide range of temperature.[18,19] However, in the group contribution correlation[19] based on previously available data, the group parameters for the ring oxygen atom and for the ring methylene group were not sufficiently robust, and the carbonyl group was missing entirely.

The purpose of the present contribution is to complement the solubility data in PHW with the results for several oxygen-containing aromatic solutes including xanthene, anthrone, xanthone, thioxanthone, 9,10-anthraquinone, and 9,10-phenanthrenequinone. Some of the solutes, namely, xanthene, anthrone, xanthone, and 9,10-anthraquinone, are important chemicals and potential pollutants so that the aqueous solubility data can be useful in themselves. Besides, the data are needed to upgrade and extend the solubility correlation mentioned above.

Table 1. Aqueous Solubilities of the Solutes x_2 and Their Standard Deviations SD as Functions of Temperature T and Pressure P

solute	T/K	P/MPa	10^9x_2	10^9SD [a]
xanthene	313.2	5.3	252	2.85
	323.2	5.3	471	18.1
	333.2	5.1	844	35.2
	343.2	5.1	1450	35.7
	353.2	5.0	2570	75.8
	363.2	5.0	4270	235
	368.2	5.0	5560	148
anthrone	313.2	5.1	345	14.2
	333.2	5.0	1060	33.8
	353.2	5.8	3180	63.0
	373.2	5.0	9490	231
	393.2	5.0	27900	748
	413.2	5.0	98900	1180
	423.2	5.0	126000	2410
xanthone	313.2	5.3	709	15.5
	333.2	5.1	1930	48.5
	353.2	5.0	5440	149
	373.2	5.0	12900	355
	393.2	5.1	37000	1160
	413.2	5.0	91300	3260
	433.2	5.0	271000	4140
thioxanthone	313.2	5.4	118	3.72
	333.2	5.2	313	14.4
	353.2	5.1	879	41.4
	373.2	5.1	2220	91.2
	393.2	5.3	6440	196
	413.2	5.2	19800	594
	433.2	5.3	55000	2830
	453.2	5.3	135000	4920
	473.2	6.4	383000	8000
9,10-anthraquinone	313.2	5.0	72.5	3.80
	333.2	5.0	205	9.79
	353.2	5.0	592	28.5
	373.2	5.1	1560	101
	393.2	5.2	4100	132
	413.2	5.0	10600	186
	433.2	5.8	29600	453
9,10-phenanthrenequinone	313.2	5.2	550	5.36
	333.2	5.0	1630	63.0
	353.2	5.0	4180	102
	373.2	5.0	10600	568
	393.2	5.0	39400	1460
	413.2	5.0	84600	1470
	433.2	5.1	255000	8540
	453.2	5.3	842000	46400
	473.2	5.4	1830000	68300

[a] Standard deviations (SD) are based on five fractions collected at each condition.

In line with our previous studies, the present data were measured along the 5 MPa isobar in the temperature interval

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Table 2. Least-Squares Estimates of the Coefficients a_1, a_2, and a_3 of Equation 1 and the Standard Deviations (SD) of the Estimates, with T_{min} and T_{max} Indicating the Minimum and the Maximum Temperatures of the Solubility Measurements, Respectively

solute	xanthene	anthrone	xanthone	thioxanthone	9,10-anthraquinone	9,10-phenanthrenequinone
T_{min}/K	313.2	313.2	313.2	313.2	313.2	313.2
T_{max}/K	368.2	423.2	433.2	473.2	433.2	473.2
a_1	−9.244	−34.33	−37.73	−42.88	−33.18	−40.32
SD a_1	4.35	10.8	5.52	2.94	3.16	6.40
a_2	−6.915	18.61	22.89	26.21	15.97	25.20
SD a_2	4.38	11.0	5.60	3.00	3.21	6.53
a_3	12.99	35.30	36.72	40.07	31.38	39.44
SD a_3	3.85	8.99	4.55	2.34	2.61	5.08

Table 3. Values of $RT^2(\partial \ln x_2/\partial T)_{P,\sigma}$/kJ·mol^{-1} Calculated from Equation 3

T/K	xanthene	anthrone	xanthone	thioxanthone	9,10-anthraquinone	9,10-phenanthrenequinone
313.2	51.0	45.8	38.8	39.4	42.1	40.2
333.2	53.1	51.7	45.0	46.0	47.3	46.8
353.2	55.3	57.5	51.1	52.7	52.5	53.3
373.2		63.4	57.2	59.3	57.8	59.9
393.2		69.3	63.3	66.0	63.0	66.5
413.2		75.1	69.4	72.7	68.2	73.0
433.2			75.5	79.3	73.4	79.6
453.2				86.0		86.1
473.2				92.7		92.7

Table 4. Solute Properties Used to Obtain the Fugacity Ratio f_2^{s0}/f_2^{l0}

solute	ΔH_2^{fus}/J·mol^{-1}	ref	T_{t2}/K	ref
xanthene	19 200	31	373.7[a]	32
anthrone	26 800	33	428.15[a]	34
xanthone	26 120	35	434.1[a,b]	36
thioxanthone	35 500	37	487.88[a]	37
9,10-anthraquinone	32 570	38	558.0[a,c]	39

[a] Normal melting point temperature. [b] Estimated with the Joback correlation. [c] Average of 10 individual data points compiled by the Thermodynamics Research Center, NIST Boulder Laboratories.

from 313 K to the solute melting point. The experimental solubilities were also used to estimate the activity coefficients of the individual solutes in their aqueous solutions at saturation.

Experimental Section

Materials. Xanthene (99 %, CAS No. 92-83-1), anthrone (97 %, CAS No. 90-44-8), xanthone (97 %, CAS No. 90-47-1), thioxanthone (97 %, CAS No. 492-22-8), 9,10-anthraquinone (97 %, CAS No. 84-65-1), and 9,10-phenanthrenequinone (> 99 %, CAS No. 84-11-7) were purchased from Sigma-Aldrich (Prague, Czech Republic). Prior to use, anthrone, xanthone, thioxanthone, and 9,10-anthraquinone were recrystallized from benzene. Analyses of calibration solutions of the purified solutes by gas chromatography/mass spectrometry (GC/MS) indicated the purities > 99 % in all cases. Benzene (99.8 %) and methylene chloride (99.8 %) were supplied by Penta (Chrudim, Czech Republic), and hexane (> 95 %) was purchased from Riedel deHaën (Prague, Czech Republic). Water was purified with a reverse osmosis system Ultra Clear UV (SG Wasseraufbereitung and Regenerierstation, Barsbüttel, Germany).

Apparatus and Procedure. The aqueous solubilities were measured by a dynamic method employing the apparatus described before.[14] Briefly, the dynamic method was employed to generate the aqueous solution of the solute at the particular temperature and pressure, and a known mass of the solution was allowed to cool to room temperature. The solute was then extracted with an organic solvent, and the organic solution was analyzed by GC/MS employing diamantane as the internal standard. Hexane was used as the organic solvent for xanthene, anthrone, and xanthone, whereas methylene chloride was used with thioxanthone, 9,10-anthraquinone, and 9,10-phenanthrenequinone. Any errors caused by the residual amount of the solute in the aqueous phase were within the experimental uncertainty as indicated by repeated aqueous−organic equilibration experiments.

The operating procedure was the same as in our previous studies of solid solubilities in PHW.[14−17] In the present work, the dimensions of fused-silica tubing used as the flow restrictor were 1.2 m in length and 75 μm i.d. The mass of individual samples of the aqueous solution ranged within (3 to 8) g, and the mass flow rate of water through the system was always less than 0.017 g·s^{-1}. An initial test of the flow-rate dependence of the measured solubility was carried out with 9,10-phenanthrenequinone at 333.2 K and 5 MPa using fused-silica restrictors of various lengths and diameters. The results of the test did not indicate any significant variation in the composition of the aqueous effluent as the flow rate of water varied within (0.008 to 0.028) g·s^{-1}. The standard uncertainty[20] in the measurement of the extraction cell temperature was ± 0.10 K, and the standard uncertainty in the measurement of pressure was ± 0.1 MPa.

GC/MS Operating Conditions. A TraceGC gas chromatograph fitted with a TriPlus AS autosampler was equipped with a DB-5 capillary column (30 m × 0.25 mm i.d., polymer film thickness 0.25 μm, J&W Scientific, Folsom, CA) and coupled to a PolarisQ mass spectrometer (TraceGC + PolarisQ, Thermo Finnigan, San Jose, CA). The carrier gas was helium (99.995 %, SIAD, Braňany u Mostu, Czech Republic); the ionization energy (EI mode) was 70 eV; and the splitless injection technique was employed with all solutes. The GC oven temperature was programmed from 323 K (6 s) at 0.17 K·s^{-1} to the final temperature (60 s). The final temperature was 468 K, 503 K, 488 K, 518 K, 508 K, and 523 K in xanthene, anthrone, xanthone, thioxanthone, 9,10-anthraquinone, and 9,10-phenanthrenequinone, respectively.

Results and Discussion

Solubility Data. The aqueous solubilities (equilibrium mole fractions, x_2) of the solutes are listed in Table 1. In most solutes, the upper temperature limits of the measurements were (5 to 15) K below the normal melting point temperature of the solute. In 9,10-anthraquinone, the measurements had to be terminated at 433.2 K (approximately 125 K below the melting point) because the outlet end of the fused silica restrictor invariably became clogged with the precipitating solute at higher temperatures of measurement. The GC/MS analyses of the organic

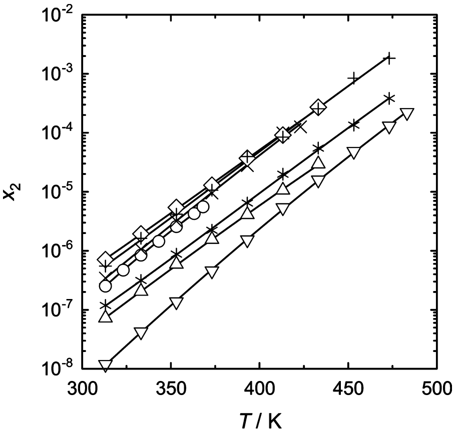

Figure 1. Aqueous solubilities of oxygenated aromatic solutes: ○, xanthene; ×, anthrone; ◇, xanthone; *, thioxanthone; Δ, 9,10-anthraquinone; +, 9,10-phenanthrenequinone. Anthracene[14] ▽ is shown for reference. The lines show the best fits of the data with eq 1.

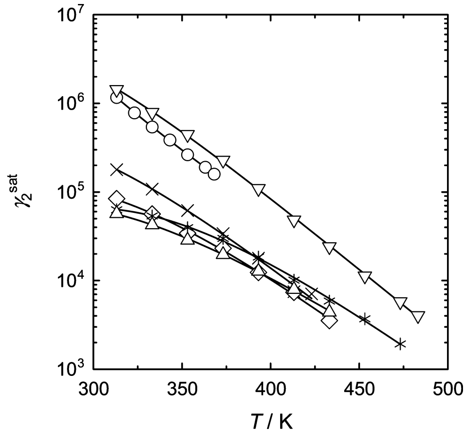

Figure 2. Estimates of activity coefficients of oxygenated aromatic solutes in saturated aqueous solutions (ΔC_{P2}/J·mol^{-1}·K^{-1} = 0): ○, xanthene; ×, anthrone; ◇, xanthone; *, thioxanthone; Δ, 9,10-anthraquinone. Anthracene[18] ▽ is shown for reference. The lines serve just to guide the eye.

extracts of the aqueous solutions did not indicate any noticeable decomposition of any of the solutes under the present experimental conditions. Considering the data in Table 2 and the standard uncertainties in temperature and pressure mentioned above, we conclude that the relative expanded uncertainty[20] in the resultant solubilities is ± 12 % (confidence level of 95 %).

Variation of Solubility with Temperature. Simple linear fits of the data from Table 1 indicate that the mean values of the relative increase in solubility with temperature, $(\partial \ln x_2/\partial T)_\sigma$, are 0.056 K^{-1}, 0.055 K^{-1}, 0.049 K^{-1}, 0.051 K^{-1}, 0.050 K^{-1}, and 0.051 K^{-1} in xanthene, anthrone, xanthone, thioxanthone, 9,10-anthraquinone, and 9,10-phenanthrenequinone, respectively. These values are similar to those reported before for PAHs.[14,15] A more detailed picture of the effect of temperature on solubility results from fitting the data from Table 1 with

$$\ln x_2 = a_1 + a_2(T_0/T) + a_3 \ln(T/T_0) \qquad (1)$$

where T_0 = 298.15 K. The fits of the data from Table 1 with eq 1 are shown in Figure 1, and the least-squares estimates of the coefficients a_1, a_2, and a_3 are listed in Table 2. In all coefficients, the ratio of the coefficient estimate to the standard deviation of the coefficient estimate can be compared to the pertinent critical values of the Student's t distribution[21] to test the hypothesis "the coefficient equals zero". In all coefficients except those of xanthene, the hypothesis is rejected at a confidence level of 98 %, indicating that the coefficients are statistically significant. The xanthene coefficient estimates are less robust than those of the other solutes because the temperature range available for the measurements with solid xanthene (55 K) was more narrow than the ranges of the other solutes (110 K at least).

Temperature dependence of solid solubility has often been used to estimate the enthalpy of solution. Starting from standard thermodynamic relationships,[22,23] one can show[14] that

$$\bar{H}_2 - H_2^{\mathrm{s0}} = RT^2\left(\frac{\partial \ln x_2}{\partial T}\right)_{P,\sigma}\left[1 + \left(\frac{\partial \ln \gamma_2}{\partial \ln x_2}\right)_{T,P}\right] \qquad (2)$$

where $\bar{H}_2$ is the partial molar enthalpy of the solute in the solution; H_2^{s0} is the molar enthalpy of the pure solid solute; R is the molar gas constant; P is the pressure; γ_2 is the Raoult law activity coefficient of the solute referred to the pure subcooled liquid solute at the particular T and P; and subscript σ denotes saturation. The values of $RT^2(\partial \ln x_2/\partial T)_{P,\sigma}$ can readily be estimated using the coefficients from Table 2

$$RT^2\left(\frac{\partial \ln x_2}{\partial T}\right)_{P,\sigma} = R(a_3T - a_2T_0) \qquad (3)$$

and they are compiled in Table 3. Equation 2 indicates, however, that these values cannot be converted to the transfer enthalpies $\bar{H}_2 - H_2^{\mathrm{s0}}$ unless the respective quotients $(\partial \ln \gamma_2/\partial \ln x_2)_{T,P}$ are known.

The only independent result we found in the literature on aqueous solubilities of the present solutes was the value of $x_2 = 1.11 \cdot 10^{-7}$ obtained from the data reported by Stovall et al.[24] for xanthene at 298.15 K and atmospheric pressure. Extrapolation of the present data for xanthene using eq 1 with the coefficients from Table 2 yields $x_2 = 9.60 \cdot 10^{-8}$. This result compares reasonably with the value obtained by Stovall et al. because the difference can partly be explained by the effect of elevated pressure in the present study.

Estimation of Activity Coefficients. The solubility x_2 of a solid solute (2) in a liquid solvent (1) is given by

$$x_2 = \frac{f_2^{\mathrm{s0}}}{\gamma_2^{\mathrm{sat}} f_2^{\mathrm{l0}}} \qquad (4)$$

where f_2^{s0} and f_2^{l0} are the fugacities of the pure solid solute and the pure subcooled liquid solute, respectively, and γ_2^{sat} is the Raoult law activity coefficient of the solute in the saturated solution. The activity coefficient is referred to the pure subcooled liquid solute at the particular temperature and pressure. Equation 4 applies if the solid phase in equilibrium with the solution is pure solute. The fugacity ratio in eq 4 can be expressed as[25]

$$\ln \frac{f_2^{\mathrm{s0}}}{f_2^{\mathrm{l0}}} = \frac{\Delta H_2^{\mathrm{fus}}}{RT_{\mathrm{t2}}}\left(1 - \frac{T_{\mathrm{t2}}}{T}\right) + \frac{\Delta C_{P2}}{R}\left(\frac{T_{\mathrm{t2}}}{T} - 1\right) - \frac{\Delta C_{P2}}{R} \ln \frac{T_{\mathrm{t2}}}{T} + \frac{(V_2^{\mathrm{s0}} - V_2^{\mathrm{l0}})P}{RT} \qquad (5)$$

where T_{t2} is the triple-point temperature of the solute; $\Delta H_2^{\mathrm{fus}}$ is the molar enthalpy of fusion of the solute at T_{t2}; ΔC_{P2} is the difference between the molar isobaric heat capacities of the pure subcooled liquid solute and the pure solid solute ($= C_{P2}^{\mathrm{l0}} - C_{P2}^{\mathrm{s0}}$); and V_2^{s0} and V_2^{l0} are the molar volumes of the pure solid solute and the pure subcooled liquid solute, respectively. Equation 5 applies if there are no solid−solid phase transitions in the pure solute within the temperature interval from T to T_{t2}. The last term on the rhs of eq 5 accounts for the effect of elevated pressure on f_2^{s0} and f_2^{l0} assuming that both the solid solute and the subcooled liquid solute are incompressible and that their respective vapor pressures are negligible with respect to the total pressure P. In the present solutes, no experimental values of ΔC_{P2} are available. Therefore, in accordance with the recommendation by Pappa et al.[26] for PAHs, the approximation $\Delta C_{P2}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1} = 0$ was adopted here, and the values of solute fugacity ratio were calculated from

$$\ln\frac{f_2^{s0}}{f_2^{l0}} \approx \frac{\Delta H_2^{\text{fus}}}{RT_{t2}}\left(1 - \frac{T_{t2}}{T}\right) + \frac{(V_2^{s0} - V_2^{l0})P}{RT} \qquad (6)$$

The molar volumes of subcooled liquid solutes were evaluated from the modified Rackett equation[27] using the critical properties estimated from the Joback correlation,[28,29] and the molar volumes of solid solutes were obtained using the correlation of Goodman et al.[30] The values and sources of ΔH_2^{fus} and T_{t2} of the solutes are listed in Table 4.

Figure 2 shows the temperature dependence of the solute activity coefficients estimated via eqs 4 and 6. Numerical values of γ_2^{sat} are available in the Supporting Information file. As one can expect, the presence of oxygen atom(s) in the solute molecule tends to make the solute less hydrophobic as compared with anthracene at the particular temperature. 9,10-Phenanthrenequinone is missing from Figure 2 because, in this solute, we have not found any published value of the enthalpy of fusion needed to convert the solubilities to activity coefficients.

Conclusion

A dynamic method with a flow-through extraction cell was employed to measure the aqueous solubilities of several oxygen-containing tricyclic aromatic solids at temperatures between 313 K and the solute melting point. The presence of oxygen atom(s) (ring, carbonyl, or both) in the solute molecule appears to make the solute less hydrophobic as compared with anthracene at the particular temperature.

Supporting Information Available:

Estimates of the activity coefficients of oxygenated aromatic solids in aqueous solutions. The estimates were obtained assuming $\Delta C_{P2}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1} = 0$ (Table S1). This material is available free of charge via the Internet at http://pubs.acs.org.

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