Solubilities of Triptycene, 9-Phenylanthracene, 9,10-Dimethylanthracene, and 2-Methylanthracene in Pressurized Hot Water at Temperatures from 313 K to the Melting Point

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Aqueous solubilities of two $C_{20}H_{14}$ isomers, triptycene (9,10-*o*-benzeno-9,10-dihydroanthracene) and 9-phenylanthracene, 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. In addition, aqueous solubilities of 2-methylanthracene and 9,10-dimethylanthracene were also obtained. The curvature of the temperature dependence of triptycene solubility differs distinctly from those for the other solutes. Although no data on aqueous solubilities of the solutes at $T > 323.15$ K were found in the literature, the results for methylanthracenes at the lower limit of the temperature range of the present measurements compare favorably with previous reports. The activity coefficients of triptycene in saturated aqueous solutions were estimated from the measured solubilities employing two different approximations for the pure solute heat capacity difference ΔC_{P2}.

Introduction

Aqueous solubility data at elevated temperatures are important in applications of water as a tunable solvent for green chemical technology.[1,2] Tunability of the solvent properties of water results from the effects of temperature and pressure on the cohesive energy density, ion product, and relative permittivity of water. Although these effects are most readily apparent in supercritical water,[3–7] they are definitely important even at lower temperatures in pressurized hot water (PHW) (= liquid water at temperatures between the normal boiling point and the critical point).

In some applications of PHW, e.g., in environmental remediation processes or in sample treatment procedures for analytical chemistry, aqueous solubility data of heavy organic nonelectrolyte solids at high temperatures can be very useful. At the present time, relatively few data sets of this kind can be found in the literature. Most previous solubility measurements in PHW were concerned with polycyclic aromatic hydrocarbons (PAHs),[8–13] and solubility data for solid tricyclic aromatic heterocycles are also available.[14] To date, there are virtually no data on solubilities in PHW of solutes with large molecules containing both aromatic and aliphatic moieties. An example of such a molecule is triptycene (9,10-*o*-benzenoanthracene, $C_{20}H_{14}$), synthesized in 1942.[15] Triptycene is a nonplanar molecule with a "paddlewheel" structure, and the triptycene skeleton has some interesting recent applications in the design of molecular machines (motors,[16] mechanisms,[17] tweezers[18]) and hydrogen storage materials.[19]

The primary purpose of this work was to measure the aqueous solubility of solid triptycene and compare it with the solubility of another $C_{20}H_{14}$ isomer, 9-phenylanthracene. Unlike the molecule of triptycene, the molecule of 9-phenylanthracene is nearly planar. We also intended to measure the aqueous solubilities of other aromatic $C_{20}H_{14}$ isomers, namely, 1,1′-binaphthyl and 2,2′-binaphthyl, but we did not succeed in securing sufficient amounts of the two compounds to carry out the measurements. The purpose was to evaluate the effect of the structural difference between triptycene and planar aromatics on aqueous solubilities and solute–water interactions. In addition to aqueous solubilities of triptycene and 9-phenylanthracene, the solubilities of 2-methylanthracene and 9,10-dimethylanthracene in PHW were also determined. Unlike the aqueous solubilities of 2-methylanthracene and 9,10-dimethylanthracene, the aqueous solubilities of triptycene and 9-phenylanthracene have not been reported yet.

Experimental Section

Materials. 9,10-Dimethylanthracene (99 %), 9-phenylanthracene (98 %), triptycene (98 %), and fluorene (> 99 %) were purchased from Sigma-Aldrich (Prague, Czech Republic). 2-Methylanthracene (> 99 %) was obtained from Fluka (Prague, Czech Republic). All solutes were used as received because the analyses of the calibration solutions of these compounds by gas chromatography/mass spectrometry (GC/MS) did not indicate the presence of any major impurities. Toluene (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 und Regenerierstation, Barsbüttel, Germany).

Apparatus and Procedure. The aqueous solubilities were measured by a dynamic method employing the apparatus described before.[13] 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 hexane, and the organic solution was analyzed by GC/MS employing fluorene as the internal standard. Any errors caused by the residual amount of the solute in the aqueous

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Table 1. GC Oven Program Settings for the Individual Solutes

	initial isotherm	duration	ramp rate	final isotherm	duration
solute	K	s	$\mathrm{K \cdot s^{-1}}$	K	s
2-methylanthracene	323	30	0.17	503	30
9,10-dimethylanthracene	323	30	0.17	523	30
9-phenylanthracene	323	30	0.17	543	60
triptycene	323	30	0.17	523	60

Table 2. 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	$10^9 x_2$	$10^9\mathrm{SD}^{a}$
2-methylanthracene	313.2	6.4	5.23	0.331
	333.2	5.1	18.6	0.891
	353.2	5.0	64.3	2.76
	373.2	5.1	256	5.30
	393.2	5.1	833	10.2
	413.2	5.1	2450	69.5
	433.2	5.4	7730	182
	453.2	5.6	30600	662
9,10-dimethylanthracene	313.2	5.3	3.27	0.165
	333.2	5.1	10.7	0.140
	353.2	5.0	41.0	0.777
	373.2	5.0	138	3.12
	393.2	5.0	507	23.9
	413.2	5.0	1710	41.6
	433.2	5.0	5280	208
	448.2	5.2	12400	491
9-phenylanthracene	313.2	5.1	0.757	0.101
	333.2	5.0	3.44	0.149
	353.2	5.0	11.6	0.640
	373.2	5.1	40.7	1.80
	393.2	5.0	171	8.10
	413.2	5.0	671	15.4
	423.2	5.0	1200	67.3
triptycene	313.2	5.1	7.57	0.269
	333.2	5.2	20.3	0.982
	353.2	5.0	60.2	1.47
	373.2	5.0	179	4.03
	393.2	5.0	526	15.4
	413.2	5.0	1770	39.0
	433.2	5.3	5780	98.7
	453.2	5.0	18100	414
	473.2	5.1	59100	2020
	493.2	5.0	174000	6890
	513.2	5.0	539000	25000

[a] Standard deviations (SD) are based on 5 fractions collected at each condition.

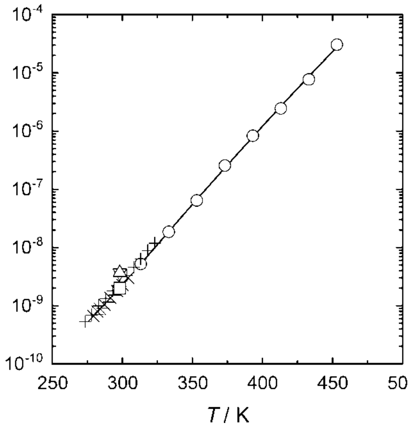

Figure 1. Aqueous solubility data of 2-methylanthracene from different sources. ▽, Mackay & Shiu;[21] ×, May et al.;[22,23] □, May et al.;[24] Δ, Yalkowsky & Valvani;[25] -, Whitehouse;[26] +, Dohányosová et al.;[27] ○, this work. The line is the best fit of the data from this work with eq 1.

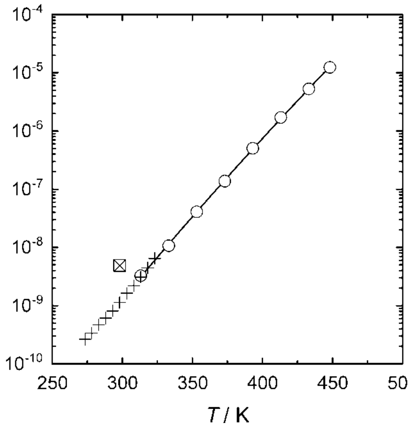

Figure 2. Aqueous solubility data of 9,10-dimethylanthracene from different sources. □, Mackay & Shiu;[21] ×, Yalkowsky & Valvani;[25] +, Dohányosová et al.;[27] ○, this work. The line is the best fit of the data from this work with eq 1.

phase were safely within the experimental uncertainty as indicated by repeated aqueous–organic equilibration experiments.

The operating procedure was the same as in the previous studies with PAHs[13] and aromatic heterocycles.[14] In the present study, 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 $\mathrm{g \cdot s^{-1}}$. An initial test of the flow-rate dependence of the measured solubility was carried out with 9-phenylanthracene 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) $\mathrm{g \cdot s^{-1}}$. 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), and the ionization energy (EI mode) was 70 eV. The GC oven temperature program was optimized for each individual solute, and the final settings employed are compiled in Table 1.

Results and Discussion

Solubility Data. The aqueous solubilities (equilibrium mole fractions, x_2) of the solutes are listed in Table 2. The upper temperature limits of the measurements were (5 to 25) K below the normal melting point temperature of the particular solute. The GC/MS analyses of the hexane 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 ± 10 % (confidence level of 95 %).

Comparison of Solubility Data with Literature Values. Figure 1 shows a comparison of the present results on aqueous solubilities of 2-methylanthracene with literature data. There is only a 10 K overlap between the temperature ranges of the measurements of Dohányosová et al.[27] and the present data.

Table 3. 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	2-methylanthracene	9,10-dimethylanthracene	9-phenylanthracene	triptycene
T_{min}/K	313.2	313.2	313.2	313.2
T_{max}/K	453.2	448.2	423.2	513.2
a_1	−40.41	−39.95	−49.07	−56.69
SD a_1	6.35	3.35	8.94	1.20
a_2	20.39	19.40	27.13	37.27
SD a_2	6.46	3.40	9.06	1.23
a_3	39.42	38.70	46.66	50.71
SD a_3	5.13	2.71	7.42	0.919

The results of this study are somewhat lower than the solubilities reported by Dohányosová et al. This finding can partly be explained by the effect of elevated pressure in the present measurements. On the other hand, the present results appear to extrapolate to what is a fair agreement with the data of May et al.[22,23] The solubilities reported by Mackay and Shiu[21] and by Yalkowsky and Valvani[25] exceed the other data at 298.15 K,[22–24,26,27] and they also exceed an estimated value that would result from extrapolation of the present measurements.

The aqueous solubilities of 9,10-dimethylanthracene are plotted in Figure 2. Here, the present data agree very well with those of Dohányosová et al.,[27] and the solubilities reported by Mackay and Shiu[21] and by Yalkowsky and Valvani[25] again exceed the data of Dohányosová[27] at 298.15 K as well as an extrapolation of the present results.

Variation of Solubility with Temperature. Simple linear fits of the data from Table 2 show that the mean values of the relative increase in solubility with temperature, $(\partial \ln x_2/\partial T)_\sigma$, are 0.061 K^{-1}, 0.062 K^{-1}, 0.067 K^{-1}, and 0.057 K^{-1} in 2-methylanthracene, 9,10-dimethylanthracene, 9-phenylanthracene, and triptycene, respectively. These values are similar to those reported before for other PAH solutes.[13] A more detailed picture of the effect of temperature on solubility results from fitting the data from Table 2 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 least-squares estimates of the coefficients a_1, a_2, and a_3 are listed in Table 3. 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[28] to test the hypothesis "the coefficient equals zero". In all coefficients, the hypothesis is rejected at a confidence level of 98 %, indicating that the coefficients are statistically significant.

Figure 3 shows the solubility data together with the fits via eq 1. The fitting lines emphasize the different directions of curvature of the anthracene[13] and triptycene plots. However, the difference in curvature between the two plots is not an artifact of the fits via eq 1. The different signs of curvature are apparent when drawing straight lines between the data points at the limits of the temperature range in the individual solutes. The vertical axis of Figure 3 has a logarithmic scale, and the solubilities of the individual solutes span over 3 or more orders of magnitude. Therefore, the opposite signs of curvature of the anthracene[13] and the triptycene plots are even invariant with respect to the relative expanded uncertainty in the solubility data given above.

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

$$x_2 = \frac{f_2^{s0}}{\gamma_2^{sat} f_2^{l0}} \qquad (2)$$

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 2 applies if the solid phase in equilibrium with the solution is pure solute. The fugacity ratio in eq 2 can be obtained from the thermochemical cycle described by Prausnitz et al.,[29]

$$\ln \frac{f_2^{s0}}{f_2^{l0}} = \frac{\Delta H_2^{fus}}{RT_{t2}}\left(1 - \frac{T_{t2}}{T}\right) + \frac{\Delta C_{P2}}{R}\left(\frac{T_{t2}}{T} - 1\right) - \frac{\Delta C_{P2}}{R} \ln \frac{T_{t2}}{T} + \frac{(V_2^{s0} - V_2^{l0})P}{RT} \qquad (3)$$

where *R* is the molar gas constant; *T* is the temperature; T_{t2} is the triple-point temperature of the solute; ΔH_2^{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 ($= C_{P2}^{l0} - C_{P2}^{s0}$); and V_2^{s0} and V_2^{l0} are the molar volumes of the pure solid solute and the pure subcooled liquid solute, respectively. The last term on the rhs of eq 3 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*. Equation 3 applies if there are no solid–solid phase transitions in the pure solute within the temperature interval from *T* to T_{t2}.

Equations 2 and 3 were used to obtain the γ_2^{sat} values of triptycene from the aqueous solubilities. For the other solutes, we did not find any data on ΔH_2^{fus} in the journal literature. The triptycene solubility data were converted to estimates of γ_2^{sat} via eqs 2 and 3 using T_{t2} = 527.18 K[30] and ΔH_2^{fus} = 30.275 kJ·mol^{-1}.[30] Since no experimental data on ΔC_{P2} are available for triptycene, two common approximations[31] of ΔC_{P2} were employed, namely, ΔC_{P2}/J·mol^{-1}·K^{-1} = 0 and $\Delta C_{P2} = \Delta S_2^{fus}$, where ΔS_2^{fus} is the entropy of fusion (= 57.43 J·mol^{-1}·K^{-1}).[30] The molar volume of subcooled liquid triptycene was evaluated from the modified Rackett equation[32] using the critical temperature and critical pressure estimated from the Joback correlation.[33,34] The molar volume of solid triptycene was obtained using the correlation of Goodman et al.[35]

Figure 4 shows the activity coefficients γ_2^{sat} obtained from the aqueous solubility data of triptycene and anthracene[13,36] assuming ΔC_{P2}/J·mol^{-1}·K^{-1} = 0. Yalkowsky[31] and later Pappa et al.[37] reported that, in PAHs, this was relatively the best approximation (as compared[37] to approximating ΔC_{P2} by the entropy of fusion and to the use of group contribution models to estimate C_{P2}^{l0} and C_{P2}^{s0}). However, the best approximation for PAHs need not necessarily provide the best approximation for the nonplanar molecule of triptycene. Figure 5 presents a comparison of the approximations ΔC_{P2}/J·mol^{-1}·K^{-1} = 0 and $\Delta C_{P2} = \Delta S_2^{fus}$ when converting aqueous solubilities of triptycene and anthracene to γ_2^{sat}. In the two solutes, the effects of the two approximations of ΔC_{P2} on the resultant values of γ_2^{sat} are very similar because the ΔS_2^{fus} values for triptycene and anthracene are very close to each other (57.43 J·mol^{-1}·K^{-1} [30]

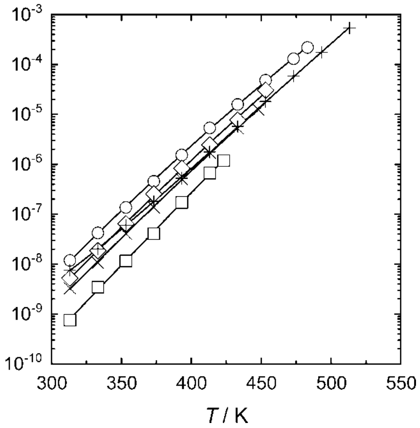

Figure 3. Experimental data on solute solubilities vs the best fits with eq 1: ◇, 2-methylanthracene; ×, 9,10-dimethylanthracene; □, 9-phenylanthracene; +, triptycene. Anthracene[13] ○ is shown for reference. The lines are the best fits with eq 1.

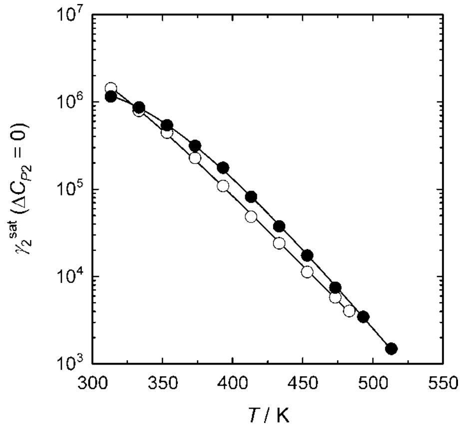

Figure 4. Solute activity coefficients in saturated aqueous solutions as calculated from eqs 2 and 3 assuming $\Delta C_{P2}/\text{J·mol}^{-1}\text{·K}^{-1} = 0$. ○, anthracene;[36] ●, triptycene.

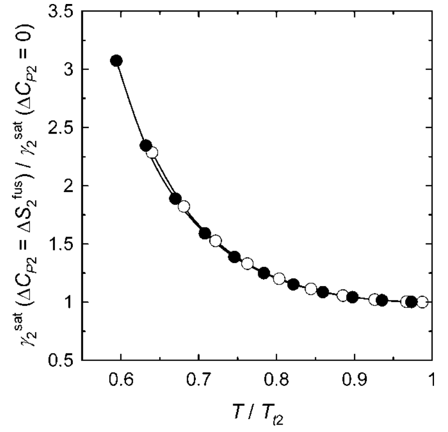

Figure 5. Relative effects of the approximations $\Delta C_{P2}/\text{J·mol}^{-1}\text{·K}^{-1} = 0$ and $\Delta C_{P2} = \Delta S_2^{\text{fus}}$ on the calculated activity coefficients. ○, anthracene; ●, triptycene.

and 59.1 $\text{J·mol}^{-1}\text{·K}^{-1}$,[38] respectively). Figure 5 illustrates the important effect of the approximation of ΔC_{P2} on the resultant value of γ_2^{sat}. As the ratio T/T_{t2} decreases below unity, the ensuing increase in importance of ΔC_{P2} is exponential.

Conclusion

A dynamic method with a flow-through extraction cell was employed to measure the solubilities of solid triptycene, 9-phenylanthracene, 9,10-dimethylanthracene, and 2-methylanthracene in pressurized hot water from 313 K to the solute melting point. Depending on temperature, the solubility of triptycene exceeded the solubility of the planar $C_{20}H_{14}$ isomer, 9-phenylanthracene, by a factor ranging from 2.6 to 10. Overall, the solubility of triptycene was close to the solubilities of methylanthracenes, approaching the solubility of 2-methylanthracene at low temperatures and the solubility of 9,10-dimethylanthracene at high temperatures. Further, the aqueous solubility of triptycene was always lower than the solubility of anthracene at the same temperature. With the current lack of reliable information on ΔC_{P2} for the two solutes, it is impossible to resolve whether the solubility difference between triptycene and anthracene comes from different pure solute fugacity ratios or from different solute–water interactions.

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