

|   |  |
|---|--|
| COMPONENTS:<br><br>(1) Dibenz[a,h]anthracene; C <sub>22</sub> H <sub>14</sub> ; [58-70-3]<br>(2) Water; H <sub>2</sub> O; [7732-18-5] | EVALUATOR:<br><br>G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.<br><br>June 1986. |
|---|--|

## CRITICAL EVALUATION:

Quantitative solubility data for dibenz[a,h]anthracene (1) in water (2) have been reported in the publications listed in Table 1. No data are available for the solubility of water in dibenz[a,h]anthracene.

TABLE 1. Quantitative Solubility Studies of Dibenz[a,h]anthracene (1) in Water (2)

| Reference                   | T/K | Method             |
|-----------------------------|-----|--------------------|
| Davis <i>et al.</i> (ref 1) | 300 | nephelometric      |
| Klevens (ref 2)             | 298 | spectrophotometric |

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. The two reported values, although obtained at slightly different temperatures, are in excellent agreement. Nevertheless there are insufficient data and the system is insufficiently well-characterized to justify a higher than Tentative classification.

TABLE 2. Tentative Solubility Values of Dibenz[a,h]anthracene (1) in Water (2)

| T/K | Solubility values                                 |   |                                 |
|-----|---|---|---------------------------------|
|     | Reported values<br>10 <sup>8</sup> g(1)/100 g sln | "Best" values<br>10 <sup>8</sup> g(1)/100 g sln | 10 <sup>11</sup> x <sub>1</sub> |
| 298 | 5.84 (ref 2)                                      | 6   | 4                               |
| 300 | 5 (ref 1)   | 5   | 3                               |

## REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
- Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.

|  |   |
|--|---|
| <b>COMPONENTS:</b><br><br>(1) Dibenz[a,h]anthracene; C <sub>22</sub> H <sub>14</sub> ; [58-70-3]<br><br>(2) Water; H <sub>2</sub> O; [7732-18-5]   | <b>ORIGINAL MEASUREMENTS:</b><br><br>Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.<br><br><i>J. Am. Chem. Soc.</i> <u>1942</u> , <i>64</i> , 108-10.   |
| <b>VARIABLES:</b><br><br>One temperature: 27°C   | <b>PREPARED BY:</b><br><br>M.C. Haulait-Pirson  |
| <b>EXPERIMENTAL VALUES:</b><br><br>The solubility of dibenz[a,h]anthracene in water at 27°C was reported to be $5 \times 10^{-7}$ g(l) L <sup>-1</sup> (2).<br>(Two identical results have been obtained)<br>With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are $5 \times 10^{-8}$ g(l)/100 g sln and $3 \times 10^{-11}$ .     |   |
| <b>AUXILIARY INFORMATION</b>   |   |
| <b>METHOD/APPARATUS/PROCEDURE:</b><br><br>The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).<br>A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1. | <b>SOURCE AND PURITY OF MATERIALS:</b><br><br>(1) Eastman Kodak Company; purified; m.p. range 266.6-266.9°C or Hoffman La Roche; m.p. range 262.7-264°C (cf. ref 2).<br><br>(2) dust-free.                              |
|  | <b>ESTIMATED ERROR:</b><br>temp. $\pm 3^\circ\text{C}$<br>soly. $\pm 10^{-7}$ g(l) dm <sup>-3</sup> (2)   |
|  | <b>REFERENCES:</b><br>1. Davis, W.W.; Parker, Jr., T.V. <i>J. Am. Chem. Soc.</i> <u>1942</u> , <i>64</i> , 101.<br>2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. <i>J. Am. Chem. Soc.</i> <u>1940</u> , <i>62</i> , 3086. |

|   |   |
|---|---|
| <b>COMPONENTS:</b><br><br>(1) Dibenz[a,h]anthracene; C <sub>22</sub> H <sub>14</sub> ; [58-70-3]<br><br>(2) Water; H <sub>2</sub> O; [7732-18-5]  | <b>ORIGINAL MEASUREMENTS:</b><br><br>Klevens, H.B.<br><br><i>J. Phys. Chem.</i> <u>1950</u> , 54, 283-98.   |
| <b>VARIABLES:</b><br><br>Temperature: 25°C  | <b>PREPARED BY:</b><br><br>M.C. Haulait-Pirson  |
| <b>EXPERIMENTAL VALUES:</b><br><br>The solubility of dibenz[a,h]anthracene in water at 25°C was reported to be $2.15 \times 10^{-9}$ mol(1) L <sup>-1</sup> sln.<br>With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are $5.84 \times 10^{-8}$ g(1)/100 g sln and $3.88 \times 10^{-11}$ . |   |
| <b>AUXILIARY INFORMATION</b>  |   |
| <b>METHOD/APPARATUS/PROCEDURE:</b><br><br>The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.  | <b>SOURCE AND PURITY OF MATERIALS:</b><br><br>(1) not specified.<br>(2) not specified.<br><br><b>ESTIMATED ERROR:</b><br><br>not specified.<br><br><b>REFERENCES:</b> |

|  |   |
|--|---|
| <b>COMPONENTS:</b><br><br>(1) Dibenz[a,h]anthracene; $C_{22}H_{14}$ ;<br>[53-70-3]<br><br>(2) Salt Water   | <b>ORIGINAL MEASUREMENTS:</b><br><br>Krasnoshchekova, R.Ya.; Pakhapill,<br>Yu.A.; Gubergrits, M.Ya.<br><br><i>Khim. Tverd. Topl.</i> <u>1977</u> , <i>11</i> ,<br>133-6.  |
| <b>VARIABLES:</b><br><br>One temperature: 25°C<br>Salinity: 6 g/kg sln (ref. 1)  | <b>PREPARED BY:</b><br><br>M. Kleinschmidt and D. Shaw  |
| <b>EXPERIMENTAL VALUES:</b><br><br>The solubility of dibenz[a,h]anthracene in salt water was reported to be 21.13 µg/L.<br><br>The corresponding mass percent and mole fraction, $x_1$ , calculated by the compilers are $2.064 \times 10^{-6}$ g(1)/100 g sln and $1.397 \times 10^{-9}$ assuming a solution density of 1.004 kg/L.   |   |
| <b>AUXILIARY INFORMATION</b>   |   |
| <b>METHOD/APPARATUS/PROCEDURE:</b><br><br>1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1-L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra. | <b>SOURCE AND PURITY OF MATERIALS:</b><br><br>Not given.<br><br><b>ESTIMATED ERROR:</b><br>temp. $\pm 1^\circ\text{C}$<br>soly. $\pm 1.14$<br>type of error not specified<br><br><b>REFERENCES:</b><br>1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. <i>Neftekhimiya</i> <u>1973</u> , <i>13</i> , 885. |