| COMPONENTS: | EVALUATOR: |
|---|---|
| (1) Styrene; $C_8H_8$; [100-42-5]<br>(2) Water; $H_2O$; [7732-18-5] | G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.<br>July 1985 |

CRITICAL EVALUATION:

Quantitative solubility data for the styrene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1. Quantitative Solubility Studies of the Styrene (1) - Water (2) System

| Reference | *T*/K | Solubility | Method |
|---|---|---|---|
| Lane (ref 1) | 298-324 | mutual | various[a] |
| Fordyce and Chapin (ref 2) | 333 | (1) in (2) | titration |
| Frilette and Hohenstein (ref 3) | 298 | (1) in (2) | unspecified |
| Andrews and Keefer (ref 4) | 298 | (1) in (2) | spectrophotometric |
| Banerjee *et al.* (ref 5) | 298 | (1) in (2) | HPLC |

[a] Chemical analysis and cloud point measurements for (1) in (2). Karl Fischer and cloud point measurements for (2) in (1).

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. SOLUBILITY OF STYRENE (1) IN WATER (2)

All the available data (ref 1-5) are listed in Table 2. At 298K the agreement among the independent measurements (ref 1,3-5) is reasonable but not sufficient to enable the average value to be Recommended.

At other temperatures, the value of Fordyce and Chapin (ref 2) at ~ 333K is very much higher than that of Lane (ref 1). Since the latter were obtained by two independent methods and, as already noted, are in fair agreement with other determinations at 298K, the datum of Fordyce and Chapin is rejected. In the absence of confirmatory studies the data at temperatures other than 298K should be regarded as very tentative.

(continued next page)

| COMPONENTS: | EVALUATOR: |
|---|---|
| (1) Styrene; $C_8H_8$; [100-42-5]<br>(2) Water; $H_2O$; [7732-18-5] | G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.<br>July 1985. |

CRITICAL EVALUATION: (continued)

TABLE 2. Tentative Values of the Solubility of Styrene (1) in Water (2)

| *T*/K | Solubility values | | |
|---|---|---|---|
| | Reported values[a] (g(1)/100g sln) | "Best" values g(1)/100g sln | $10^5\ x_1$ |
| 283 | 0.29* (ref 1) | 0.029 | 5.0 |
| 293 | 0.030* (ref 1) | 0.030 | 5.2 |
| 298 | 0.033* (ref 1), 0.022 (ref 3), 0.030 (ref 4), 0.016 (ref 5) | 0.025 ± 0.006[b] | 4.3 |
| 303 | 0.034* (ref 1) | 0.034 | 5.9 |
| 313 | 0.040* (ref 1) | 0.040 | 6.9 |
| 323 | 0.046* (ref 1) | 0.046 | 8.0 |
| 333 | 0.053* (ref 1), 0.95 (ref 2)[c] | 0.053 | 9.2 |

[a] Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the author's two data sets, followed by averaging.

[b] Average (± $\sigma_n$) of all data; $\sigma_n$ has no statistical significance.

[c] At *T* = 333.5K, value rejected: see text.

## 2. THE SOLUBILITY OF WATER (2) IN STYRENE (1)

The solubility of water in styrene has been reported in only one study (ref 1) and thus no Critical Evaluation is possible. The interested user is referred to the relevant data sheet for the experimental solubility values.

## REFERENCES

1. Lane, W.H. *Ind. Eng. Chem. Anal. Ed.* 1946, *18*, 295-6.
2. Fordyce, R.G.; Chapin, E.C. *J. Am. Chem. Soc.* 1947, *69*, 581-3.
3. Frilette, V.J.; Hohenstein, W.P. *J. Polym. Sci.* 1948, *3*, 22-31.
4. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
5. Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. *Env. Sci. Technol.* 1980, *14*, 1227-9.

**COMPONENTS:**

(1) Styrene; $C_8H_8$; [100-42-5]

(2) Water; $H_2O$; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Lane, W.H.

*Ind. Eng. Chem. Anal. Ed.* 1946, *18*, 295-6.

**VARIABLES:**

Temperature: 7-65°C

**PREPARED BY:**

A. Maczynski and Z. Maczynska

**EXPERIMENTAL VALUES:**

Solubility of styrene in water

| $t$/°C | g(1)100 g sln | $10^5x_1$ (compiler) |
|---|---|---|
| (a) Formaldehyde - Sulfuric Acid Reagent Method | | |
| 7 | 0.029 | 5.0 |
| 24 | 0.033 | 5.7 |
| 32 | 0.036 | 6.2 |
| 40 | 0.040 | 6.9 |
| 51 | 0.045 | 7.8 |
| (b) Cloud Point Method | | |
| 15 | 0.025 | 4.3 |
| 25 | 0.031 | 5.3 |
| 44 | 0.040 | 6.9 |
| 49 | 0.045 | 7.8 |
| 56 | 0.050 | 8.6 |
| 65 | 0.058 | 10.0 |

## AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

(a) The solubility of (1) in (2) was determined by means of the formaldehyde-sulfuric acid reagent, ref (1). The value shown for 7°C is the mean of three determinations, and the value for 25°C is the mean of two determinations; all other data are single determinations only.
(b) The cloud point exhibited by this system appeared to be very sharp, as the samples passed from a state in which they were cloudy within 1°C. The cloud point data are averages of from two to eight separate determinations. Cloud points at 0.025 g(1)/100 g solution were very faint.

**SOURCE AND PURITY OF MATERIALS:**

(1) source not specified; fresh samples; used as received.

(2) not specified.

**ESTIMATED ERROR:**

temp. (b) ± 0.5°C (from two to eight determinations)

**REFERENCES:**

1. Morris, H.E.; Stiles, R.B.; Lane, W.H. *Ind. Eng. Chem. Anal. Ed.* 1946, *18*, 294.

**COMPONENTS:**

(1) Styrene; $C_8H_8$; [100-42-5]

(2) Water; $H_2O$; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Lane, W.H.

*Ind. Eng. Chem. Anal. Ed.* 1946, *18*, 295-6.

**VARIABLES:**

Temperature: 6-51°C

**PREPARED BY:**

A. Maczynski and Z. Maczynska

**EXPERIMENTAL VALUES:**

Solubility of water in styrene

| $t$/°C | g(2)/100 g sln | $10^3x_2$ (compiler) |
|---|---|---|
| (a) Karl Fischer Reagent Method | | |
| 6 | 0.032 | 1.8 |
| 24 | 0.066 | 3.8 |
| 31 | 0.084 | 4.8 |
| 40 | 0.101 | 5.8 |
| 51 | 0.123 | 7.1 |
| (b) Cloud Point Method | | |
| 14 | 0.040 | 2.3 |
| 27 | 0.060 | 3.5 |
| 34 | 0.080 | 4.6 |
| 40 | 0.100 | 5.7 |
| 45 | 0.120 | 6.9 |

## AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

(a) A large sample of (1) containing a slight excess of (2) was shaken at a given temperature and then allowed to stand in a water bath at this temperature for 24 hr to ensure complete separation of the two phases before withdrawal of sample of the rich phase for titration of the water present with the Karl Fischer reagent.
(b) Duplicate determinations gave cloud points agreeing within 1°C, except in the case of 0.120 g(1)/100 g solution where the agreement was within about 3°C. Cloud points at 0.040 (1)/100 g solution were very faint. No more details were reported.

**SOURCE AND PURITY OF MATERIALS:**

(1) source not specified; fresh samples; used as received.

(2) not specified.

**ESTIMATED ERROR:**

soly. (a) ± 1.5% (from two determinations)
temp. (b) ± 1 to ± 3°C.

**REFERENCES:**

**COMPONENTS:**

(1) Styrene; $C_8H_8$; [100-42-5]

(2) Water; $H_2O$; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Fordyce, R.G.; Chapin, E.C.

*J. Am. Chem. Soc.* 1947, *69*, 581-3.

**VARIABLES:**

One temperature: 60.3°C

**PREPARED BY:**

A. Maczynski

**EXPERIMENTAL VALUES:**

The solubility of styrene in water at 60.3 C was reported to be 0.96 g(1)/100 g(2).

The corresponding mass percent and mole fraction, $x_1$, calculated by the compiler are 0.95 g(1)/100 g sln and $1.66 \times 10^{-3}$.

AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

Into two stoppered 50 mL Erlenmeyer flasks were weighed two 25.000 g portions of (2). The flasks were placed in a water-bath regulated to 60.3 ± 0.02°C. Component (1) was added a drop at a time to the water samples by means of a calibrated micro-pipet and the flasks agitated after each addition. The saturation point was taken at the first appearance of the turbidity and the amount of (1) was calculated from the number of drops added.

**SOURCE AND PURITY OF MATERIALS:**

(1) Dow Chemical Co, N-100; redistilled.

(2) Not specified.

**ESTIMATED ERROR:**

temp. ±0.02°C

soly. ±0.05 g(1)/100 g sln

**REFERENCES:**

**COMPONENTS:**

(1) Styrene; $C_8H_8$; [100-42-5]

(2) Water; $H_2O$; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Frilette, V.J.; Hohenstein, W.P.

*J. Polym. Sci.* 1948, *3*, 22-31.

**VARIABLES:**

One temperature: 25°C

**PREPARED BY:**

A. Maczynski and Z. Maczynska

**EXPERIMENTAL VALUES:**

The solubility of styrene in water at 25°C was reported to be 0.022 g(1)/100 g sln.

The corresponding mole fraction, $x_1$, value calculated by the compilers is $3.8 \times 10^{-5}$.

## AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The saturated solutions of (1) in (2) were prepared in two different ways. In the first method, conjugated solutions were prepared by shaking together excess (1) with (2) and allowing the layers to separate; the aqueous layer was then analyzed for (1). To avoid the possibility of contaminating the aqueous phase by small suspended droplets a second method was utilized; a cellophane sack, filled with (2) was completely submerged in a beaker containing (2); a layer of (1) was then floated on top of (2) in the beaker. After 48 hr at 25°C, the sack was retrieved and the contents carefully removed and analyzed.

The method of analysis was not described.

**SOURCE AND PURITY OF MATERIALS:**

(1) not specified.

(2) distilled.

**ESTIMATED ERROR:**

Not specified.

**REFERENCES:**

**COMPONENTS:**

(1) Styrene; $C_8H_8$; [100-42-5]

(2) Water; $H_2O$; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Andrews, L.J.; Keefer, R.M.

*J. Am. Chem. Soc.* 1950, *72*, 5034-7.

**VARIABLES:**

One temperature: 25°C

**PREPARED BY:**

A. Maczynski and Z. Maczynska

**EXPERIMENTAL VALUES:**

The solubility of styrene in water at 25°C was reported to be 0.030 g(1)/100 g sln.

The corresponding mole fraction, $x_1$, calculated by the compilers is $5.19 \times 10^{-5}$.

AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

**SOURCE AND PURITY OF MATERIALS:**

(1) Eastman Kodak Co. white label; distilled shortly before use; 1 wt % of hydroquinone added as stabilizer before distillation; b.p. 76 C (78 mm Hg).

(2) Not specified.

**ESTIMATED ERROR:**

Not specified.

**REFERENCES:**

| COMPONENTS: | ORIGINAL MEASUREMENTS: |
|---|---|
| (1) Styrene; $C_8H_8$; [100-42-5]<br>(2) Water; $H_2O$; [7732-18-5] | Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C.<br>*Environ. Sci. Technol.* 1980, *14*, 1227-9. |
| **VARIABLES:** | **PREPARED BY:** |
| One temperature: 25°C | G.T. Hefter |

**EXPERIMENTAL VALUES:**

The solubility of styrene in water was reported to be 1.54 x $10^{-3}$ mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction ($x_1$) solubilities, calculated by the compiler, are 0.0160 g(1)/100 g sln and 2.77 x $10^{-5}$ respectively.

## AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of styrene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25 ± 0.2°C with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to 25 ± 0.3°C, following which aliquots of the solution were removed for analysis by high-performance liquid chromatography using a Waters M6000A instrument fitted with a $C_{18}$ Bondapak column. The mobile phase was a mixture of methanol/water or acetonitrile/water. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.

**SOURCE AND PURITY OF MATERIALS:**

(1) Aldrich; purity not specified.

(2) Distilled.

**ESTIMATED ERROR:**

Temperature: ±0.2°C

Solubility: ±5.7% rel. (representing one std. dev.)

**REFERENCES:**