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| COMPONENTS: (1) Undecane; C ₁₁ H ₂₄ ; [1120-21-4] (2) Water; H ₂ O; [7732-18-5] | EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. December 1985. |
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CRITICAL EVALUATION:

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

TABLE 1: Quantitative Solubility Studies of the Undecane (1) - Water (2) System

| Reference | T/K | Solubility | Method |
|--|---------|------------|--------------|
| Schatzberg (ref 1) | 298,313 | (2) in (1) | Karl Fischer |
| McAuliffe (ref 2) | 298 | (1) in (2) | GLC |
| Krasnoshchekova and Gubergrits (ref 3) | 298 | (1) in (2) | GLC |

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

For convenience further discussion of this system will be divided into two parts.

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

The available data for the solubility of undecane in water are listed in Table 2.

TABLE 2: Solubility Values of Undecane (1) in Water (2)

| T/K | Solubility values | | |
|-----|--|---|---------------------------------|
| | Reported values 10 ⁷ g(1)/100g sln | "Best" value (± σ _n) 10 ⁷ g(1)/100g sln | 10 ¹⁰ x ₁ |
| 298 | 4.4 (ref 2), 3.6 (ref 3) | 4.0 ± 0.4 ^a | 4.6 ^a |

^a Order of magnitude only, see text; obtained by averaging.

Although the agreement between the two studies (ref 2,3) is very good considering the very low solubility involved, both values are very much lower than expected from an extrapolation of *n*-alkane solubilities. This may be due (ref 2) to micelle formation. The available data must therefore be considered as Doubtful. The extrapolated value of 1.4 × 10⁻⁶ g(1)/100g sln (x₁ = 1.6 × 10⁻¹⁰) may be more realistic.

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| <p>COMPONENTS:</p> <p>(1) Undecane; $C_{11}H_{24}$; [1120-21-4]</p> <p>(2) Water; H_2O; [7732-18-5]</p> | <p>EVALUATOR:</p> <p>G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.</p> <p>December 1985.</p> |
| <p>CRITICAL EVALUATION: (continued)</p> <p>2. SOLUBILITY OF WATER (2) IN UNDECANE (1)</p> <p>As only one publication (ref 1) reports solubility data for water in undecane no Critical Evaluation is possible. However, it may be noted that the data of Schatzberg (ref 1) are generally reliable. The interested user is referred to the relevant Data Sheet for the experimental values.</p> <p>REFERENCES</p> <ol style="list-style-type: none">1. Schatzberg, P. <i>J. Phys. Chem.</i> <u>1963</u>, <i>67</i>, 776-9.2. McAuliffe, C. <i>Science</i> <u>1969</u>, <i>163</i>, 478-9.3. Krasnoshchekova, P.Y.; Gubergrits, M.Y. <i>Neftekhimiya</i> <u>1973</u>, <i>13</i>, 885-7. | |

| COMPONENTS: (1) Undecane; $C_{11}H_{24}$; [1120-21-4] (2) Water; H_2O ; [7732-18-5] | ORIGINAL MEASUREMENTS: Schatzberg, P. <i>J. Phys. Chem.</i> <u>1963</u> , <i>67</i> , 776-9. | | | | | | | | | |
|---|---|-----------------------|---------------------|----------------------|----|-----------------|----------------------|----|------------------|-----------------------|
| VARIABLES: Temperature: 25-40°C | PREPARED BY: M.C. Haulait-Pirson | | | | | | | | | |
| EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of water in undecane</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>mg(2)/kg sln</u></th> <th style="text-align: center;"><u>x₂</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">25</td> <td style="text-align: center;">69^a</td> <td style="text-align: center;">6.0×10^{-4}</td> </tr> <tr> <td style="text-align: center;">40</td> <td style="text-align: center;">130^b</td> <td style="text-align: center;">11.3×10^{-4}</td> </tr> </tbody> </table> <p>a, b See "Estimated Error"</p> | | <u>t/°C</u> | <u>mg(2)/kg sln</u> | <u>x₂</u> | 25 | 69 ^a | 6.0×10^{-4} | 40 | 130 ^b | 11.3×10^{-4} |
| <u>t/°C</u> | <u>mg(2)/kg sln</u> | <u>x₂</u> | | | | | | | | |
| 25 | 69 ^a | 6.0×10^{-4} | | | | | | | | |
| 40 | 130 ^b | 11.3×10^{-4} | | | | | | | | |
| AUXILIARY INFORMATION | | | | | | | | | | |
| METHOD/APPARATUS/PROCEDURE: <p>(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.</p> | SOURCE AND PURITY OF MATERIALS: <p>(1) Phillips Petroleum Co.; research grade; 99.33 mole%; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range.</p> <p>(2) distilled and deionized.</p> ESTIMATED ERROR: temp. $\pm 0.02^\circ\text{C}$ soly. a) 0-6%; b) 0-2% (deviations from the mean) | | | | | | | | | |
| REFERENCES: | | | | | | | | | | |

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| COMPONENTS: (1) Undecane; $C_{11}H_{24}$; [1120-21-4] (2) Water; H_2O ; [7732-18-5] | ORIGINAL MEASUREMENTS: McAuliffe, C. <i>Science</i> <u>1969</u> , <i>163</i> , 478-9. |
| VARIABLES: One temperature: 25°C | PREPARED BY: F. Kapuku |
| EXPERIMENTAL VALUES: The solubility of undecane in water at 25°C was reported to be 0.0044 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 4.4×10^{-7} g(1)/100 g sln and 5.07×10^{-10} . | |
| AUXILIARY INFORMATION | |
| METHOD/APPARATUS/PROCEDURE: (1) was equilibrated with (2). Glass vials were filled with the saturated aqueous phase. Half of water was then displaced and replaced by air. The vials were then sealed and shaken for 2 minutes. The gas phase was then displaced through the sample loop of a gas chromatograph for analyzing for hydrocarbon content. | SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) distilled. ESTIMATED ERROR: soly. ± 0.0018 mg(1)/kg(2) REFERENCES: |

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| COMPONENTS: (1) Undecane; $C_{11}H_{24}$; [1120-21-4] (2) Water; H_2O ; [7732-18-5] | ORIGINAL MEASUREMENTS: Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. <i>Neftekhimiya</i> <u>1973</u> , 13, 885-7. |
| VARIABLES: One temperature: 25°C | PREPARED BY: A. Maczynski |
| EXPERIMENTAL VALUES: <p>The solubility of undecane in water at 25°C was reported to be $\pi_1 = 4.10 \times 10^{-10}$.</p> <p>The corresponding mass percent calculated by the compiler is 3.6×10^{-7} g(1)/100 g sln.</p> | |
| AUXILIARY INFORMATION | |
| METHOD/APPARATUS/PROCEDURE: <p>A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigorously stirred magnetically for 10-12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.</p> | SOURCE AND PURITY OF MATERIALS: (1) source not specified; CP reagent; purity not specified. (2) distilled. ESTIMATED ERROR: not specified. REFERENCES: |

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| COMPONENTS: (1) Undecane; $C_{11}H_{24}$; [1120-21-4] (2) Seawater | ORIGINAL MEASUREMENTS: Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. <i>Neftekhimiya</i> <u>1973</u> , 13, 885-8. |
| VARIABLES: One temperature: 25°C Salinity: 6 g/kg sln | PREPARED BY: M. Kleinschmidt |
| EXPERIMENTAL VALUES: <p>The solubility of undecane in seawater was reported to be 1.0×10^{-6} g(1)/100 g sln. and the corresponding mole fraction, $x_1 = 1.2 \times 10^{-9}$.</p> | |
| AUXILIARY INFORMATION | |
| METHOD/APPARATUS/PROCEDURE: <p>A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.</p> | SOURCE AND PURITY OF MATERIALS: (1) "chemically pure" (2) distilled water plus salt mixture. |
| | ESTIMATED ERROR: not specified. |
| | REFERENCES: |