

COMPONENTS: (1) 1-Hexene; C ₆ H ₁₂ ; [592-41-6] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. November 1984
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CRITICAL EVALUATION:

Quantitative solubility data for the system 1-hexene (1) and Water (2) have been reported in the publications listed in Table 1.

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

Reference	T/K	Solubility	Method
Englin <i>et al.</i> (ref 1)	303	(2) in (1)	analytical
McAuliffe (ref 2)	298	(1) in (2)	GLC
Leinonen and Mackay (ref 3)	298	(1) in (2)	GLC
Budantseva <i>et al.</i> (ref 4)	293	mutual	GLC, Karl Fischer

Solubilities of 1-hexene in dilute aqueous HNO₃ solutions have also been reported (ref 5) but will not be considered in this Evaluation.

The original data in all of these publications (ref 1-5) 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. THE SOLUBILITY OF 1-HEXENE (1) IN WATER (2)

The solubility data for 1-hexene in water are given in Table 2.

TABLE 2: Recommended (R) and Tentative Values of the Solubility of 1-Hexene (1) in Water (2)

T/K	Solubility Values		
	Reported values 10 ³ g(1)/100g sln	"Best" values (± σ _n) ^a 10 ³ g(1)/100g sln	10 ⁵ x ₁
293	5 (ref 4)	1	1
298	5.0 (ref 2), 5.54 (ref 3)	5.3 ± 0.3 (R)	1.14 (R)

^a"Best" values obtained by averaging where possible; σ_n has no statistical significance.

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CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN 1-HEXENE (1)

The solubility data for water in 1-hexene are listed in Table 3. As data have not been obtained under comparable conditions they must be classified as "Tentative". However, it can be noted that in (other) well characterised systems the data of Englin *et al.* (ref 1) at $T < 300\text{K}$ are usually close to "Recommended" values. The data of Budantseva *et al.* (ref 4) on the other hand are often high.

TABLE 3: Tentative values of the Solubility
of Water (2) in 1-Hexene (1)

T/K	Solubility values	
	g(2)/100g sln	$10^3 x_2$
293	0.029 (ref 4)	1.4
303	0.048 (ref 1)	2.2

REFERENCES

- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6
- McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
- Leinonen, P.J.; Mackay, D. *Can. J. Chem. Eng.* 1973, *51*, 230-3.
- Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. *Zh. Fiz. Khim.* 1976, *50*, 1344; Deposited doc., VINITI 438-76.
- Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* 1972, *17*, 328-9.

COMPONENTS: (1) 1-Hexene; C ₆ H ₁₂ ; [592-41-6] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. <i>Khim. Tekhnol. Topl. Masel</i> <u>1965</u> , 10, 42-6.
VARIABLES: One temperature: 30°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES: The solubility of water in 1-hexene at 30°C was reported to be 0.0477 g(2)/100 g sln. The corresponding mole fraction, x_2 , calculated by the compilers is 2.23×10^{-3} .	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: Not specified. REFERENCES:

COMPONENTS: (1) 1-Hexene; C_6H_{12} ; [592-41-6] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: McAuliffe, C. <i>J. Phys. Chem.</i> <u>1966</u> , <i>70</i> , 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES: <p>The solubility of 1-hexene in water at 25°C was reported to be $50 \text{ g(1)}/10^6 \text{ g(2)}$.</p> <p>The corresponding mass percent and mole fraction, x_1, calculated by the compilers are $0.0050 \text{ g(1)}/100 \text{ g sln}$ and 9.2×10^{-6}.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.</p>	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. ESTIMATED ERROR: temp. $\pm 1.5 \text{ K}$ soly. $1.2 \text{ g(1)}/10^6 \text{ g(2)}$ (standard deviation of mean) REFERENCES:

<p>COMPONENTS:</p> <p>(1) 1-Hexene; C₆H₁₂; [592-41-6]</p> <p>(2) Water; H₂O; [7732-18-5]</p>	<p>ORIGINAL MEASUREMENTS:</p> <p>Natarajan, G.S.; Venkatachalam, K.A. <i>J. Chem. Eng. Data</i> <u>1972</u>, 17, 328-9.</p>
<p>VARIABLES:</p> <p>One temperature: 25°C</p>	<p>PREPARED BY:</p> <p>M.C. Haulait-Pirson, G.T. Hefter</p>
<p>EXPERIMENTAL VALUES:</p> <p>The solubility of 1-hexene in water was reported to be 7.781×10^{-4} mol L⁻¹ at 25°C.^a Assuming a solution density of 1.00 g mL⁻¹ the corresponding mass percent and mole fraction (x_1) solubilities calculated by the compilers are respectively, 0.00654 g(1)/100 g sin and 1.40×10^{-5}.</p> <p>Solubility data are also presented as a function of temperature in various salt solutions.</p> <p>^a It should be noted that although the authors state that the solubility refers to "water" the context in the paper is ambiguous and the data were probably obtained in 0.001 mol L⁻¹ HNO₃ solution</p>	
<p>AUXILIARY INFORMATION</p>	
<p>METHOD/APPARATUS/PROCEDURE:</p> <p>15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard procedures.</p>	<p>SOURCE AND PURITY OF MATERIALS:</p> <p>(1) Matheson, Coleman and Bell; 99%</p> <p>(2) Not specified</p> <p>ESTIMATED ERROR:</p> <p>Temp. ± 0.05 K</p> <p>Soly. not specified.</p> <p>REFERENCES:</p>

COMPONENTS: (1) 1-Hexene; C ₆ H ₁₂ ; [592-41-6] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Leinonen, P.J.; Mackay, D. <i>Can. J. Chem. Eng.</i> <u>1973</u> , <i>51</i> , 230-3.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES: <p>The solubility of 1-hexene in water at 25°C was reported to be 55.4 mg(1) dm⁻³ sln.</p> <p>The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00554 g(1)/100 g sln and 1.18×10^{-5}.</p> <p>The compiler's calculation assumes a solution density of 1.00 g mL⁻¹.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>A mixture of (1) and (2) was equilibrated at 25 ± 0.1°C for a minimum of 12 hrs in a 200-mL Teflon-stoppered vessel (25 cm long and 3.5 cm across) with gentle shaking, allowed to settle for 6 hrs and tested for the absence of emulsion (Tyndall effect). The aqueous and organic phases were analyzed by glc (with internal standardization) on a Hewlett-Packard Model 700 instrument equipped with a 15% SE-30 on 60/80 mesh acid-washed (CH₃)₂Cl₂Si-treated Chromosorb P column (steel capillary 10 ft x 0.125 inch). The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analyzed by glc.</p>	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Co. research grade, 99+ mole%; used as received. (2) doubly distilled. ESTIMATED ERROR: temp. ± 0.1 K soly. 30 mg(1) dm ⁻³ (two standard deviations) REFERENCES:

COMPONENTS: (1) 1-Hexene; C ₆ H ₁₂ ; [592-41-6] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. <i>Zh. Fiz. Khim.</i> 1976, 50, 1344. <i>Deposited doc.</i> 1976, VINITI 438-76.
VARIABLES: One temperature: 20 °C	PREPARED BY: A. Maczynski
EXPERIMENTAL VALUES: The solubility of 1-hexene in water at 20°C was reported to be $x_1 = 1 \times 10^{-5}$. The corresponding mass percent calculated by the compiler is 0.005 g(1)/100 g sln. The solubility of water in 1-hexene at 20°C was reported to be $x_2 = 0.0016$. The corresponding mass percent calculated by the compiler is 0.029 g(2)/100 g sln.	
AUXILIARY INFORMATION	
METHOD/Apparatus/Procedure: The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by Karl Fischer reagent method.	SOURCE AND PURITY OF MATERIALS: (1) source not specified; pure or analytical reagent grade; purity <99.9%. (2) not specified. ESTIMATED ERROR: Not specified. REFERENCES: