COMPONENTS:	EVALUATOR:
(1) 3-Methylhexane; C_7H_{16}; [589-34-4]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.
(2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	November 1984

CRITICAL EVALUATION:

Quantitative solubility data for the system 3-methylhexane (1) and water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the System 3-Methylhexane (1) - Water (2)

Reference	T/K	Solubility	Method
Polak and Lu (ref 1)	273,298	mutual	GLC, Karl Fischer
Price (ref 2)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 3)	298	(1) in (2)	GLC

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. THE SOLUBILITY OF 3-METHYLHEXANE (1) IN WATER (2)

Although the solubility of 3-methylhexane in water has been reported in three publications (ref 1,2,3) the datum of Krzyzanowska and Szeliga (ref 3) does not appear to be independent of that of Price (ref 2) and is thus excluded from consideration. The remaining 298K data, of Price (ref 2) and Polak and Lu (ref 1), are in poor agreement. In the absence of confirmatory studies the average of these two studies: $(3.8\pm0.9)\times10^{-4}$ g(1)/100g sln, $x_1=6.8\times10^{-7}$, is regarded as the "Tentative" solubility of 3-methylhexane in water. However, it may be noted that Polak and Lu's values for other hydrocarbon water systems are often higher and Price's values often lower than "Recommended" values.

2. THE SOLUBILITY OF WATER (2) IN 3-METHYLHEXANE (1)

The solubility of water in 3-methylhexane has been reported only by Polak and Lu (ref 1) ans so no critical evaluation can be made. The interested user is referred to the relevant Data Sheet for solubility values. However, it can be noted that the data of Polak and Lu are generally close to "Recommended" values in well characterized systems.

REFERENCES

1. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
2. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
3. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylhexane; C_7H_{16}; [589-34-4] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
VARIABLES:	**PREPARED BY:**
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 3-methylhexane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0[a]	5.24[c]	9.41×10^{-7}
25[b]	4.95[c]	8.89×10^{-7}

Solubility of water in 3-methylhexane

t/°C	mg(2)/kg sln	x_2 (compiler)
0[a]	25[d]	1.39×10^{-4}
25[b]	74[e]	4.12×10^{-4}

[a-e] see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

temp. a) ± 0.02 K; b) ± 0.01 K
soly. c) ± 1.7%; d) ± 4.7%;
e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylhexane; C_7H_{16}; [589-34-4] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylhexane in water at 25°C and at system pressure was reported to be 2.64 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 2.64×10^{-4} g(1)/100 g sln and 4.75×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1 K
soly. ± 0.08 mg(1)/kg(2)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylhexane; C_7H_{16}; [589-34-4] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)*, 1978, *12*, 413-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylhexane in water at 25°C was reported to be 2.64 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 2.64×10^{-4} g(1)/100 g sln and 4.75×10^{-7}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.10 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Heptane; C_7H_{16}; [142-82-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H_2O; [7732-18-5]	October 1986.

CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Fuhner (ref 1)	289	(1) in (2)	cloud point
Milligan (ref 2)	298	(1) in (2)	partition coefficient
Black *et al.* (ref 3)	283-298	(2) in (1)	radiotracer
Booth and Everson (ref 4)	298	(1) in (2)	residue volume
Durand (ref 5)	289	(1) in (2)	cloud point
McCants *et al.* (ref 6)	311	(1) in (2)	cloud point
Guseva and Parnov (ref 7)	345-460	(1) in (2)[a]	not specified
Schatzberg (ref 8)	298	(2) in (1)	Karl Fischer
Englin *et al.* (ref 9)	273-323	(2) in (1)	analytical
Zel'venskii *et al.* (ref 10)	296	(2) in (1)	radiotracer
Connolly (ref 11)	568-628[b]	(1) in (2)	cloud point
McAuliffe (ref 12)	298	(1) in (2)	GLC
Nelson and DeLigny (ref 13)	277-318	(1) in (2)	GLC
Ghanem *et al.* (ref 14)	296	(2) in (1)	radiotracer
Krasnoshchekova and Gubergrits (ref 15)	298	(1) in (2)	GLC
Polak and Lu (ref 16)	273,298	mutual	GLC, analytical
Budantseva *et al.* (ref 17)	293-313	mutual	not specified
Price (ref 18)	298-424	(1) in (2)	GLC
Korenman and Aref'eva (ref 19)	293	(1) in (2)	titration
Krzyzanowska and Szeliga (ref 20)	298	(1) in (2)	GLC
Bittrich *et al.* (ref 21)	298-313[c]	mutual	GLC
Rudakov and Lutsyk (ref 22)	298	(1) in (2)	partition coefficient
Jonsson *et al.* (ref 23)	288-308	(1) in (2)	partition coefficient

a Solubility in D_2O also reported.

b Pressure also varied.

c Temperature not specified for solubility of (1) in (2).

The original data in all the publications listed in Table 1 are compiled in the Data Sheets immediately following this Critical Evaluation with the exception of that of Milligan (ref 2) who employed a petroleum fraction of unspecified composition. Phase studies and critical phenomena have also been reported at elevated pressures (ref 25,26) but contain insufficient data to justify compilation.

(continued next page)