COMPONENTS:	EVALUATOR:
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7]	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 2,4-dimethylpentane (1) and water (2) are reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies for the 2,4-Dimethylpentane (1) - Water (2) System

Reference	*T*/K	Solubility	Method
McAuliffe (ref 1)	298	(1) in (2)	GLC
McAuliffe (ref 2)	298	(1) in (2)	GLC
Polak and Lu (ref 3)	273,298	mutual	GLC, Karl Fischer
Price (ref 4)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 5)	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 in two parts.

1. THE SOLUBILITY OF 2,4-DIMETHYLPENTANE (1) IN WATER (2)

Solubility data for 2,4-dimethylpentane in water (ref 2,4) are listed in Table 2 with the following exceptions. The datum of Krzyzanowska and Szeliga (ref 5) has been excluded because it does not appear to be independent of that of Price (ref 4). The earlier datum of McAuliffe (ref 1) is presumably superceded by his later determination (ref 2) and has also been excluded.

The 298K datum of Polak and Lu (ref 3) is considerably higher (*ca.* 25% relative) than other reported values (ref 2,4). Furthermore, the increase in solubility between 298 and 273K, as for other hydrocarbons investigated by these authors, is unusually large. The data of Polak and Lu (ref 3) are therefore rejected.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7]	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: (continued)

TABLE 2: Recommended (*R*) Value of the Solubility of 2,4-Dimethylpentane (1) in Water (2)

T/K	Solubility values		
	Reported values $10^4 g(1)/100g$ sln	"Best" values ($\pm \sigma_n$)[a] $10^4 g(1)/100g$ sln	$10^7 x_1$
298	4.06 (ref 2), 4.4 (ref 4)	4.2 ± 0.2 (*R*)	7.6 (*R*)

"Best" values obtained by averaging; σ_n has no statistical significance.

2. THE SOLUBILITY OF WATER (2) IN 2,4-DIMETHYLPENTANE (1)

The solubility of water in 2,4-dimethylpentane has been reported only by Polak and Lu (ref 3) and thus 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. McAuliffe, C. *Nature* 1963, *200*, 1092-3.

2. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.

3. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.

4. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.

5. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *Nature (London)* 1963, *200*, 1093-3.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,4-dimethylpentane in water at 25°C was reported to be 3.62 mg (1)/kg sln (0.00362 g(1)/100 g sln).
The corresponding mole fraction, x_1, calculated by the compiler, is 6.5×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

20-50 mL of (1) was added to (2) and vigorously shaken or stirred several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was directly injected into the gas chromatograph fitted with a suitable fractionator to absorb water. A hydrogen-flame ionization detector was used.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+% purity; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5 K
soly. 0.10 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,4-dimethylpentane in water at 25°C was reported to be 4.06 mg (1)/kg sln (0.00406 g(1)/100 g sln).
The corresponding mole fraction, x_1, calculated by the compiler, is 7.3×10^{-7}.
The same value is also reported in ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250 mL glass 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. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 µL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+% purity; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5 K
soly. 0.29 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

1. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* 1964, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (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 2,4-dimethylpentane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0[a]	6.50[c]	1.17×10^{-6}
25[b]	5.50[c]	9.88×10^{-7}

Solubility of water in 2,4-dimethylpentane

t/°C	mg(2)/kg sln	x_2 (compiler)
0[a]	31[d]	1.73×10^{-4}
25[b]	81[e]	4.51×10^{-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) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (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 2,4-dimethylpentane in water at 25°C and at system pressure was reported to be 4.41 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 4.41×10^{-4} g(1)/100 g sln and 7.92×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 0.05 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dimethylpentane, C_7H_{16}; [108-08-7] (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 2,4-dimethylpentane in water at 25°C was reported to be 4.41 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated by compiler are 4.41×10^{-4} g(1)/100 g sln and 7.92×10^{-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:

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

REFERENCES: