COMPONENTS:	EVALUATOR:
(1) 2,2,5-Trimethylhexane; C_9H_{20}; [3522-94-9] (2) Water; H_2O; [7732-18-5]	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.

CRITICAL EVALUATION:

Quantitative solubility data for the 2,2,5-trimethylhexane (1) and water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2,2,5-Trimethylhexane (1) - Water (2) System

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

The original data in both 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. SOLUBILITY OF 2,2,5-TRIMETHYLHEXANE (1) IN WATER (2)

All the available data on the solubility of 2,2,5-trimethylhexane in water are summarized in Table 2.

At 298K, the only temperature where comparison is possible, the values of McAuliffe (ref 1) and Polak and Lu (ref 2) are in poor agreement (Table 2). The only other value available is that of Polak and Lu at 273K. Thus all solubility values must be regarded as very Tentative in the absence of confirmatory studies.

TABLE 2: Tentative Values of the Solubility of 2,2,5-Trimethylhexane (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	$10^7 x_1$
273	1.79 (ref 2)	0.8	1.1
298	1.15 (ref 1), 0.54 (ref 2)	0.8 ± 0.3	1.1

[a] Obtained by averaging where appropriate; σ_n has no statistical signigicance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,2,5-Trimethylhexane; C_9H_{20}; [3522-94-9] (2) Water; H_2O; [7732-18-5]	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.

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN 2,2,5-TRIMETHYLHEXANE (1)

Only the data of Polak and Lu (ref 2) are available for the solubility of water in 2,2,5-trimethylhexane and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental values; however, it may be noted that the data of Polak and Lu (ref 2) are generally reliable.

REFERENCES

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

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,5-Trimethylhexane; C_9H_{20}; [3522-94-9] (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 2,2,5-trimethylhexane in water at 25°C was reported to be 1.15 mg (1)/kg sln.

The corresponding mole fraction, x_1, calculated by the compiler, is 1.62×10^{-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°C
soly. 0.008 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) 2,2,5-Trimethylhexane; C_9H_{20}; [3522-94-9] (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 2,2,5-trimethylhexane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0[a]	0.79[c]	1.11×10^{-7}
25[b]	0.54[c]	7.58×10^{-8}

Solubility of water in 2,2,5-trimethylhexane

t/°C	mg(2)/kg sln	x_2 (compiler)
0[a]	25[d]	1.78×10^{-4}
25[b]	75[d]	5.34×10^{-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°C; b) ± 0.01°C
soly. c) ± 4%; d) ± 4.7%;
e) ± 3.1% (mean)

REFERENCES: