COMPONENTS:	EVALUATOR:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5]	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-methylpentane (1) and water (2) have been reported in the publications listed in Table 1.

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

Reference	T/K	Solubility	Method
Connolly (ref 1)	573-628[a]	(1) in (2)	cloud-point
McAuliffe (ref 2)	298	(1) in (2)	GLC
Leinonen and Mackay (ref 3)	298	(1) in (2)	GLC
Polak and Lu (ref 4)	273,298	mutual	GLC, Karl Fischer
Price (ref 5)	298-423	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 6)	298	(1) in (2)	GLC

[a] At elevated pressures, p = 14-70 MPa

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

Connolly (ref 1) has reported solubilities of (1) in (2) at elevated pressures (Table 1) and determined an upper critical solution temperature of 625K at 31 MPa. However, as no other data are available under comparable conditions, no critical evaluation of his results can be made. The interested user is referred to the relevant Data Sheets for experimental values. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF 2-METHYLPENTANE (1) IN WATER (2)

The solubility data for 2-methylpentane in water are listed in Table 2 and plotted in Figure 1 with the exceptions noted below.

The datum of Krzyzanowska and Szeliga (ref 6) has been excluded because it does not appear to be independent of that of Price (ref 5). The data of Connolly (ref 1) have already been discussed above.

The datum of Polak and Lu (ref 4) at 298K is somewhat higher than those reported by others (ref 2, 3, 5). Also their value at 273K, as with other hydrocarbons investigated by these authors, shows an unusually large increase over the value at 298K. Their data are therefore rejected.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (2) Water; H_2O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. November 1984

CRITICAL EVALUATION: (continued)

At temperatures other than 298K only the data of Price (ref 5) are available and thus must be considered "Tentative".

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

T/K	Solubility values		
	Reported values[a] 10^3g(1)/100g sln	"Best" values (± σ_n)[b] 10^3g(1)/100g sln	$10^6 x_1$
298	1.38 (ref 2), 1.42 (ref 3), 1.30 (ref 5)	1.37 ± 0.05 (*R*)	2.87 (*R*)
303	1.3* (ref 5)	1.3	2.7
313	1.4* (ref 5)	1.4	2.9
323	1.5* (ref 5)	1.5	3.1
343	1.7* (ref 5)	1.7	3.6
363	2.3* (ref 5)	2.3	4.8
383	3.6* (ref 5)	3.6	7.5
403	6.8* (ref 5)	6.8	14
423	11.6* (ref 5)	12	25

[a] Values marked with an asterisk (*) obtained by graphical interpolation of original measurements by the Evaluators.

[b] "Best" values obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (2) Water; H_2O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. November 1984

CRITICAL EVALUATION: (continued)

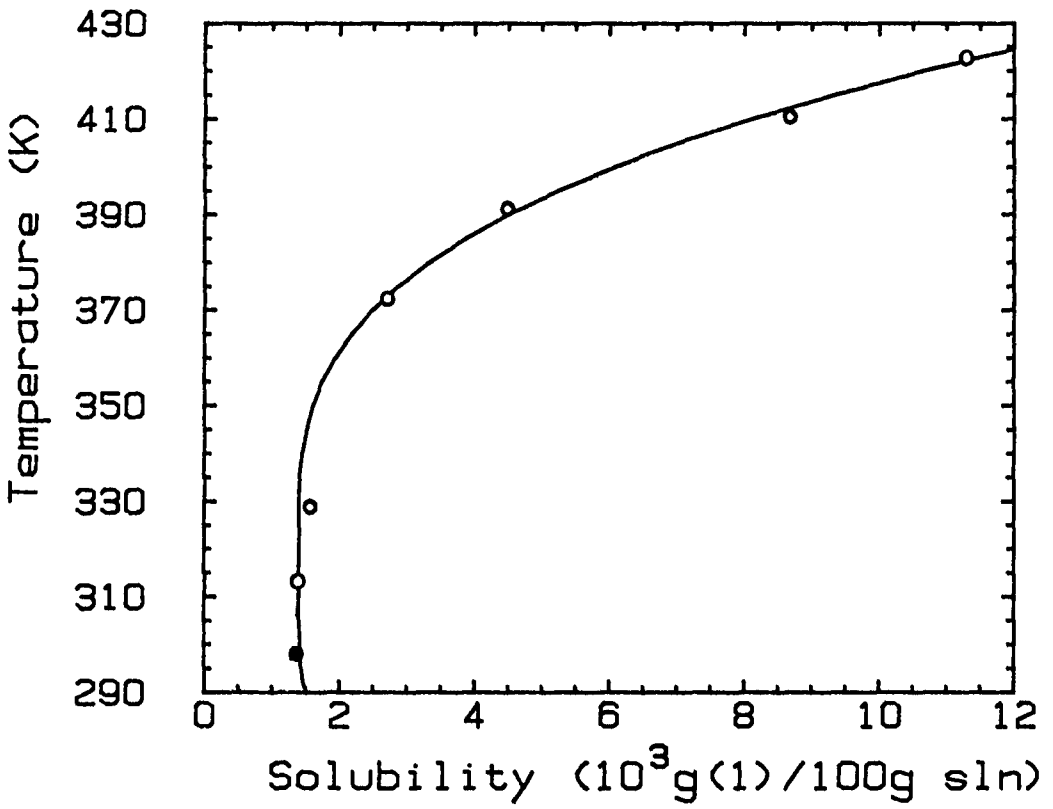

FIGURE 1. Solubility of 2-methylpentane in water: ref 5 (o); average of ref 2, 3 and 5 (●).

2. THE SOLUBILITY OF WATER (2) IN 2-METHYLPENTANE

The solubility of water in 2-methylpentane has been reported only by Polak and Lu (ref 4) and thus no Critical Evaluation can be made. However, it can be noted that the data of these authors are generally close to "Recommended" values in well characterized systems. The interested user is referred to the appropriate data sheet for solubility values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5]	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)

REFERENCES

1. Connolly, J.F. *J. Chem. Eng. Data* 1966, *11*, 13-6.
2. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
3. Leinonen, P.K.; Mackay, D. *Can. J. Chem. Eng.* 1973, *51*, 230-3.
4. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
5. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
6. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

ACKNOWLEDGEMENT

The Evaluators thank Dr Brian Clare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (2) Water; H_2O; [7732-18-5]	Connolly, J.F. *J. Chem. Eng. Data* 1966, *11*, 13-6.
VARIABLES: Temperature: 300-355°C Pressure: 140-700 atm	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 2-methylpentane in water

t/°C	p/atm	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
300	140	14.18	1.1	0.0023
	275	27.86	1.3	0.0027
	475	48.12	1.3	0.0027
	700	70.91	1.3	0.0027
330	160	16.21	1.8	0.0038
	185	18.74	2.7	0.0058
	215	21.78	3.9	0.0084
	245	24.82	4.0	0.0086
	300	30.39	4.2	0.0091
	410	41.53	4.1	0.0089
	500	50.65	3.7	0.0080
340	210	21.27	4.5	0.0097
	235	23.80	5.4	0.0118
	265	26.84	6.3	0.0138
	300	30.39	6.9	0.0152
	370	37.48	6.4	0.0140
	485	49.13	5.3	0.0116

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The cloud point method was used. Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected, until either a cloud or a small portion of a second phase appeared at the top of the cell. Then mercury was injected to change the pressure, more (1) was injected and the procedure was repeated.	(1) Phillips reagent grade; better than 99.8%; used as received. (2) distilled and deaerated.
	ESTIMATED ERROR: temp. ± 0.02 K press. ± 2 atm (accuracy)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5]	Connolly, J.F.
(2) Water, H_2O; [7732-18-5]	*J. Chem. Eng. Data* 1966, *11*, 13-6

t/°C	p/atm	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
350	230	23.30	7.1	0.0157
	240	24.31	8.2	0.0183
	260	26.34	10.4	0.0237
	275	27.86	11.6	0.0267
	290	29.38	12.5	0.0290
	310	31.40	12.8	0.0297
	335	33.94	12.5	0.0290
	365	36.97	11.6	0.0267
	405	41.03	10.5	0.0239
355	245	24.82	13.0	0.0303
	245	24.82	14.9	0.0353
	250	25.32	17.4	0.0421
	250	25.32	21.0	0.0526
	385	39.00	37.4	0.1109
	380	38.49	35.1	0.1015
	380	38.49	32.8	0.0925
	380	38.49	30.2	0.0829
	380	38.49	27.4	0.0731
	380	38.49	24.3	0.0628
	385	39.00	21.0	0.0526
	385	39.00	17.3	0.0419

COMMENTS AND ADDITIONAL DATA:

Upper critical solution temperature: 352°C at p = 310 atm.

The uncertainty in the CST is about 2°C and that of the corresponding pressure about 10 atm.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (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-methylpentane in water at 25°C was reported to be 13.8 mg (1)/kg sln (0.00138 g(1)/100 g sln).

The corresponding mole fraction, x_1, calculated by the compiler, is 2.88×10^{-6}.

The same value is also reported in refs 1 and 2.

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. 0.9 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

1. McAuliffe, C. *Nature (London)* 1963, *200*, 1092.
2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* 1964, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (2) Water; H_2O; [7732-18-5]	Leinonen, P.J.; Mackay, D. *Can. J. Chem. Eng.* 1973, *51*, 230-3.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2-methylpentane in water at 25°C was reported to be 14.2 mg(l)dm^{-3} sln.
With the assumption of a solution density of 1.00 g cm^{-3}, the corresponding mass percent is 0.00142 g(l)/100 g sln and the corresponding mole fraction, x_1, is 3.0 x 10^{-6} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was equilibrated for at least 12 hrs in a 200 mL Teflon stoppered vessel with gentle shaking. The solution was allowed to settle for 6 hrs and the aqueous phase was tested (Tyndall effect). Both phases were analysed by the gas chromatographic technique of internal standardization. The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analysed by GLC. The instrument was a Hewlett-Packard model equipped with a flame ionization detector.	(1) Phillips Petroleum Co.; research grade; purity 99%+; used without further purification. (2) doubly distilled.
	ESTIMATED ERROR: temp. ± 0.1 K soly. ± 1 mg(l)dm^{-3} sln
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (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-methylpentane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0[a]	19.45[c]	4.06×10^{-6}
25[b]	15.7[c]	3.28×10^{-6}

Solubility of water in 2-methylpentane

t/°C	mg(2)/kg sln	x_2 (compiler)
0[a]	29[d]	1.39×10^{-4}
25[b]	90[e]	4.31×10^{-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-Methylpentane; C_6H_{14}; [107-83-5] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	**PREPARED BY:**
Temperature: 25-149.5°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of 2-methylpentane in water at system pressure

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
25.0	13.0 ± 0.2	0.00130	2.72
40.1	13.8 ± 0.2	0.00138	2.88
55.7	15.7 ± 0.9	0.00157	3.28
99.1	27.1 ± 0.9	0.00271	5.67
118.0	44.9 ± 2.9	0.00449	9.39
137.3	86.8 ± 1.6	0.00868	18.15
149.5	113.0 ± 7.0	0.01130	23.62

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Room-temperature solubilities were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and insured saturation (in 2 to 4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of the gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1 K
soly. range of values given above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (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-methylpentane in water at 25°C was reported to be 13.00 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.0013 g(1)/100 g sln and 2.72×10^{-6}.

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:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: soly. 0.4 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES: