COMPONENTS:	EVALUATOR:
(1) Cyclopentane; C_5H_{10}; [287-92-3]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H_2O; [7732-18-5]	September 1984

CRITICAL EVALUATION:

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

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

Reference	*T*/K	Solubility	Method
Guseva and Parnov (ref 1)	326-472	(1) in (2)	synthetic
Englin *et al.* (ref 2)	273-313	(2) in (1)	analytical
McAuliffe (ref 3)	298	(1) in (2)	GLC
Pierotti and Liabastre (ref 4)	278-318	(1) in (2)	GLC
Price (ref 5)	298-426	(1) in (2)	GLC

The original data in all of these publications, along with the datum of Krzyzanowska and Szeliga (ref 6) are compiled in the Data Sheets immediately following this Critical Evaluation. However, the latter have not been included in this Evaluation as they do not appear to be independent of those of Price (ref 5). For convenience, further discussion of this system will be divided into two parts.

1. THE SOLUBILITY OF CYCLOPENTANE (1) IN WATER (2)

The various solubility data for cyclopentane in water are listed in Table 2. Because of the large discrepancies amongst the data and the small data base it is not possible at this stage for the Evaluator to decide on "Tentative" solubility values. The data are further discussed on the next page.

TABLE 2: Solubility of Cyclopentane (1) in Water (2)[a]

T/K	Reported solubilities, g(1)/100 g sln
278	0.0339 (ref 4)
288	0.0342 (ref 4)
298	0.0156 (ref 3), 0.0342 (ref 4), 0.0160 (ref 5)
303	0.0160 (ref 5)
313	0.035* (ref 4), 0.0163*(ref 5)
333	0.050* (ref 1), 0.0185*(ref 5)
353	0.075* (ref 1), 0.0230*(ref 5)
373	0.110* (ref 1), 0.029* (ref 5)
393	0.160* (ref 1), 0.040* (ref 5)
413	0.260* (ref 1), 0.062* (ref 5)
433	0.385* (ref 1)
453	0.67* (ref 1)
473	1.4* (ref 1)

[a] Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original measurements in the Data Sheets.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1984.

CRITICAL EVALUATION: (continued)

The solubilities in Table 2 fall into two markedly differing groups with the data of Guseva and Parnov (ref 1) and Pierotti and Liabastre (ref 4) approximately twice as high as those of McAuliffe (ref 3) and Price (ref 5). Interestingly, in spite of the disagreement, the two data sets show a similar temperature dependence (Figure 1). Application of the van't Hoff equation to these data gives ΔH^{∞}_{sln} = -2.5 (ref 4) and -2.8 (ref 5) kJ mol^{-1} which is typical for hydrocarbons in water (ref 7). However, the corresponding $\Delta C^{\infty}_{p,sln}$ values (~ -10 J K^{-1} mol^{-1}) are too negative by about 300 J K^{-1} mol^{-1} (ref 7).

Pierotti and Liabastre (ref 4) have previously noted inconsistency between their solubilities and those of McAuliffe (ref 3) for a variety of hydrocarbons. They claimed that lower solubilities are obtained by using, as McAuliffe did, a pre-absorbing column on the GLC to remove water. However, Price's GLC values (ref 5) tend to support McAuliffe's data and it should be noted that Pierotti and Liabastre's results have been found to differ markedly from "Recommended" values in a number of well-characterised systems (e.g. the benzene-water system). On the other hand, the only non-GLC data available (ref 1) are in reasonable agreement with Pierotti and Liabastre's results. This system clearly requires thorough re-investigation to resolve existing anomalies.

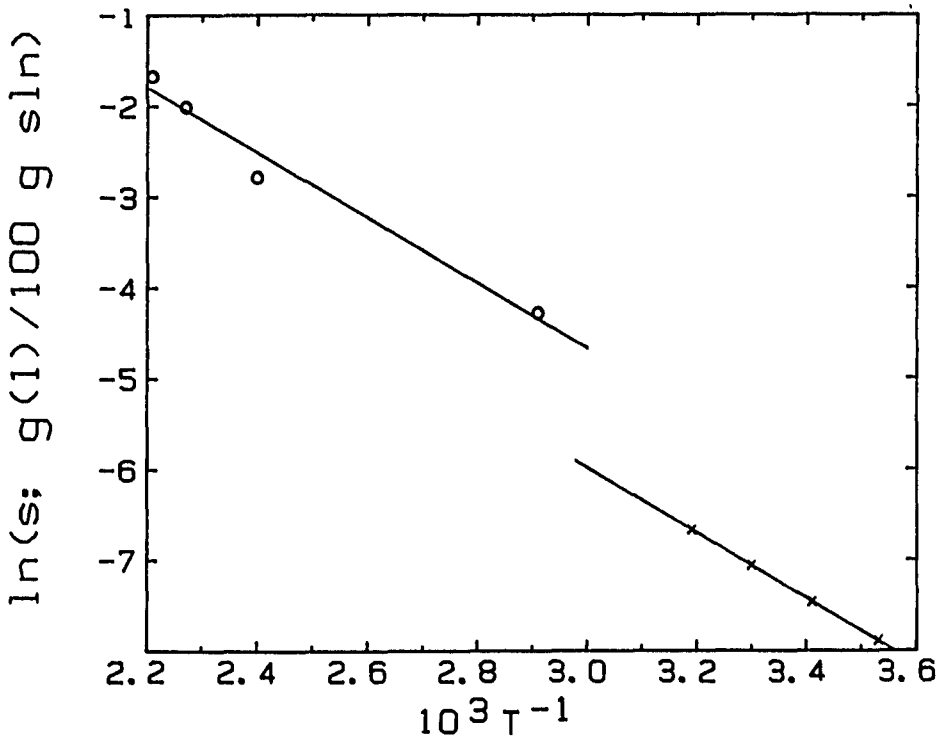

FIGURE 1. Solubility of cyclopentane (1) in water as a function of temperature: Ref 4 (X); Ref 5 (O). Data plotted as $\ell n\ s$ *vs.* T^{-1} for representational convenience.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Cyclopentane; C_5H_{10}; [287-92-3]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1984.
(2) Water; H_2O; [7732-18-5]	

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN CYCLOPENTANE

The solubility of water in cyclopentane has been reported in only one publication: Englin *et al.* (ref 2), and thus no Critical Evaluation can be made. The interested user is referred to the appropriate data sheet following this Critical Evaluation. However, it should be noted that in a number of well-characterised systems where comparison is possible (e.g. the benzene-water system) the data of Englin *et al.* are generally reliable at low temperatures but are usually much higher than "Recommended" values above 300 K.

REFERENCES

1. Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ., Khim.* 1964, *19*, 77-8.
2. Englin, B.A.; Plate, A.F.; Tugolikov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
3. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
4. Pierotti, R.A.; Liabastre, A.A. *Structure and properties of water solutions*. U.S. Nat. Tech. Inform. Serv., PB Rep. 1972, No.21163, 113 pp.
5. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
6. Krzyzanowska, T.; Szeliga, J. *Nafta Katowice* 1978, *34*, 413-7.
7. Gill, S.J.; Nichols, N.F.; Wadso, I. *J. Chem. Thermodyn.* 1976, *8*, 445-52.

ACKNOWLEDGEMENTS

The Evaluator thanks Dr Brian Clare for regression analyses and graphics and Dr Marie-Claire Haulait-Pirson for comments.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3]	Guseva, A.N.; Parnov, E.I.
(2) Water; H_2O; [7732-18-5]	*Vestn. Mosk. Univ. Khim.* 1964, *19*, 77-8.
VARIABLES:	**PREPARED BY:**
Temperature: 53-198.5°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclopentane in water

t/°C	g(1)/100 g(2)	g(1)/100 g sln (compiler)	$10^4 x_1$ (compiler)
53	0.0427	0.0427	1.10
117	0.151	0.151	3.87
166	0.436	0.434	11.12
198.5	1.288	1.271	32.57

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the measurements were made in sealed glass tubes, as reported in ref 1. No more details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* 1963, *18*, 76.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
VARIABLES: Temperature: 0-40°C	**PREPARED BY:** A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in cyclopentane

t/°C	g(2)/100 g sln	$10^4 x_2$ (compiler)
0	0.0046	1.79
10	0.0086	3.35
20	0.0142	5.53
30	0.0249	9.69
40	0.0398	15.48

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours 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:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (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 cyclopentane in water at 25°C was reported to be 156 mg(1)/kg sln, (0.0156 g/100 g sln).

The corresponding mole fraction, x_1, calculated by the compiler, is 4.0×10^{-5}.

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. ± 1.5K
soly. 9 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	Pierotti, R.A.; Liabastre, A.A. "Structure and properties of water solutions" U.S. Nat. Tech. Inform. Serv., PB Rep., 1972, No. 21163, 113 pp.
VARIABLES:	PREPARED BY:
Temperature: 278.26-318.36 K	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclopentane in water

T/ K	g(1)/100 g sln	$10^3 x_1$	$10^4 x_1$ (corrected by compiler)
278.26	0.03386 ± 0.00087	0.8697	0.8697
288.36	0.03417 ± 0.00102	0.8777	0.8777
298.26	0.03419 ± 0.00067	0.8782	0.8782
308.36	0.03685 ± 0.00110	0.9465	0.9465
318.36	0.03415 ± 0.00100	0.8772	0.8772

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

10 mL of (2) were placed along with 4-10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in a rotating basket and rotated for 24 hours. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 hours. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Matheson, Coleman & Bell, 90.8%; used as received.

(2) laboratory distilled water.

ESTIMATED ERROR:

soly.: standard deviation from at least 15 measurements are given above.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	**PREPARED BY:**
Temperature: 25-153.1°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of cyclopentane in water at system pressure

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^5 x_1$ (compiler)
25.0	160 ± 2.0	0.0160	4.11
40.1	163 ± 3.0	0.0163	4.19
55.7	180 ± 7.0	0.0180	4.62
99.1	296 ± 16.0	0.0296	7.61
118.0	372 ± 15.0	0.0372	9.56
137.3	611 ± 9.0	0.0611	15.70
153.1	792 ± 74.0	0.0792	20.36

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

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (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 cyclopentane in water at 25°C was reported to be 160.0 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.0160 g (1)/100 g sln and 4.11×10^{-5}.

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. 4.0 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES: