- (1) Cyclopentene; C₅H₈; [142-24-0]
- (2) Water; H₂O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Australia.

November 1984.

CRITICAL EVALUATION:

Quantitative solubility data for the solubility of cyclopentene (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of Cyclopentene (1) in Water (2)

Reference	T/K	Method
McAuliffe (ref 1)	298	GLC
Pierotti and Liabastre (ref 2)	298,308	GLC

Solubilities of cyclopentene have also been reported in various aqueous salt solutions (ref 3) but will not be considered in this Evaluation. No solubility data appear to have been reported for the solubility of (2) in (1).

The reported solubilities of (1) in (2) are listed in Table 2. The results are in poor agreement, those of Pierotti and Liabastre (ref 2) being about three times higher than those of McAuliffe (ref 1). These results are typical of a wide variety of hydrocarbon-water systems investigated by these authors. In general the results of McAuliffe are in good agreement with other literature values in well-investigated systems (e.g. benzene in $\rm H_2O$) whereas those of Pierotti and Liabastre are substantially higher. This situation is discussed in greater detail in the Critical Evaluation of the cyclopentane-water system. For the present system, in the absence of confirmatory studies, the data of Pierotti and Liabastre are not rejected but they should be regarded as order-of-magnitude values only. The datum of McAuliffe may be considered as "Tentative".

TABLE 2: Solubility Values of Cyclopentene (1) in Water (2)

	Reported values	"Best" value lpha	
	g(1)/100g sln	g(1)/100g sln	10 ⁴ x ₁
298	0.0535 (ref 1), 0.165 (ref 2)	0.054	1.4
308	0.175 (ref 2)		

- (1) Cyclopentene; C₅H₈; [142-24-0]
- (2) Water; H₂O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Australia. November 1984.

CRITICAL EVALUATION: (continued)

REFERENCES

- 1. McAuliffe, C. J. Phys. Chem. 1966, 70, 1267-75.
- 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.
- Natarajan, G.S.; Venkatachalam, K.A. J. Chem. Eng. Data 1972, 17, 328-9.

COMPONENTS: (1) Cyclopentene; C₅H₈; [142-29-0]

(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, 70, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski, Z. Maczynska, and

A. Szafranski

EXPERIMENTAL VALUES:

The solubility of cyclopentene in water at 25°C was reported to be $535 \text{ g}(1)/10^6 \text{ g}(2)$.

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.0535 g(1)/100 g sln and 1.41 x 10^{-4} .

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250-mL 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. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum or Columbia Chemical; used as received.
- (2) distilled.

ESTIMATED ERROR:

temp. ± 1.5 K soly. 20 g(1)/10⁶ g(2) (standard deviation of mean)

REFERENCES:

- (1) Cyclopentene; C₅H₈; [142-29-0]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Natarajan, G.S.; Venkatachalam, K.A. J. Chem. Eng. Data 1972, 17, 328-9.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of cyclopentene in water was reported to be 8.978×10^{-3} mol L⁻¹ at 25°C.^a Assuming a solution density of 1.00 g mL⁻¹ the corresponding mass percent and mole fraction (x_1) solubilities, calculated by the compilers, are respectively 0.0611 g(1)/100 g sln and 1.62 \times 10⁻⁴.

Solubility data are also presented as a function of temperature in various salt solutions.

 a It should be noted that although the authors state that the solubility refers to "water" the context in the paper is ambiguous and the data were probably obtained in 0.001 mol ${\tt L}^{-1}$ HNO3 solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard procedures.

SOURCE AND PURITY OF MATERIALS:

- (1) Prepared by dehydration of cyclopentanol and then washed, dried, and fractionated. Purity (not specified) was determined by chromatography.
- (2) Not specified.

ESTIMATED ERROR:

Temp. ± 0.05 K Soly. not specified.

REFERENCES:

- (1) Cyclopentene; C₅H₈; [142-29-0]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Pierotti, R.A.; Liabastre, A.A.

"Structure and properties of water solutions." U.S. Nat. Tech. Inform. Serv., PB Rep., 1972, No. 21163, 113 p.

VARIABLES:

Temperature: 298.26-308.36 K

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclopentene in water

<i>T/</i> K	g(1)/100 g sln	$\frac{10^3 x_1}{}$
298.26	0.1645 ± 0.0049	0.4350
308.36	0.1748 ± 0.0044	0.4623

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 the 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) K & K Laboratories, Inc.; 95-99%; used as received.
- (2) laboratory distilled water.

ESTIMATED ERROR:

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

REFERENCES: