COMPONENTS:	EVALUATOR:
(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H_2O; [7732-18-5]	November 1984.

CRITICAL EVALUATION:

Quantitative solubility data for the system 1,3,5-cycloheptatriene (1) and water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of 1,3,5-Cycloheptatriene (1) in Water (2)

Reference	T/K	Solubility	Method
Englin *et al.* (ref 1)	293-323	(2) in (1)	analytical
McAuliffe (ref 2)	298	(1) in (2)	GLC
Pierotti and Liabastre (ref 3)	278-318	(1) in (2)	GLC

The original data in 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 1,3,5-CYCLOHEPTATRIENE (1) IN WATER (2)

Solubility values of (1) in (2) are listed in Table 2 and plotted in Figure 1. The data at 298 K are in reasonable agreement. However, it should be noted that the results of Pierotti and Liabastre (ref 2) are generally higher than "Recommended" values in well characterised systems (e.g. benzene in water). Their results at temperatures other than 298 K should be regarded with some caution.

TABLE 2: Tentative Values for the Solubility of 1,3,5-Cycloheptatriene (1) in Water (2)

T/K	Solubility values		
	Reported values[a] 10^2 g(1)/100 g sln	"Best" values ($\pm \sigma_n$)[b] 10^2 g(1)/100 g sln	$10^3 x_1$
278	5.80* (ref 3)	5.8	1.1
288	6.64* (ref 3)	6.6	1.3
298	6.20 (ref 2), 6.69* (ref 3)	6.4 ± 0.2	1.25
308	7.40* (ref 3)	7.4	1.4
318	7.63* (ref 3)	7.6	1.5

[a] Values marked with an asterisk (*) obtained by the Evaluator by graphical intrapolation of original data.

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

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2] (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)

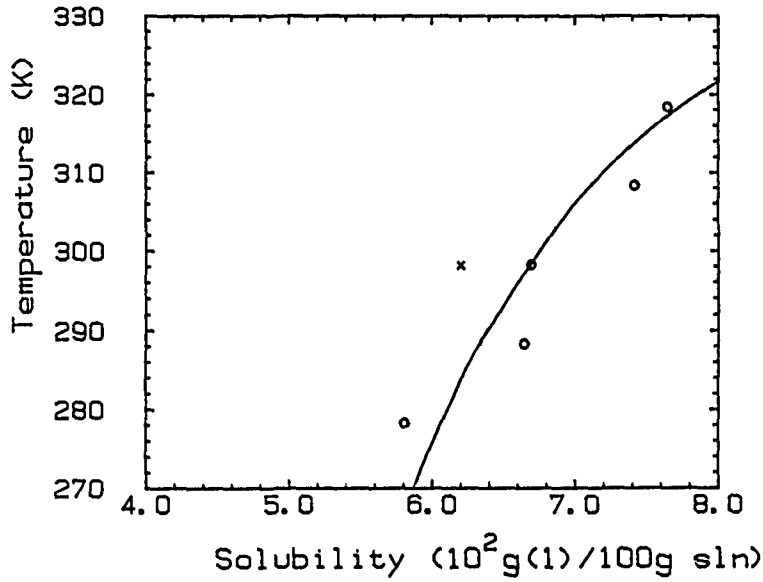

FIGURE 1. Solubility of 1,3,5-cycloheptatriene (1) in water: ref 2 (x); ref 3 (o).

2. THE SOLUBILITY OF WATER (2) IN 1,3,5-CYCLOHEPTATRIENE (1)

The solubility of water in 1,3,5-cycloheptatriene has been reported only by Englin *et al.* (ref 1) and so no Critical Evaluation can be made. The interested user is referred to the appropriate Data Sheet for solubility values. However, it should be noted that the data of Englin *et al.* are generally reliable at lower temperatures but are high when T > 300 K.

REFERENCES

1. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.

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

3. 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.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2] (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:	**PREPARED BY:**
Temperature: 30-50°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in 1,3,5-cycloheptatriene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
30	0.0630	3.21
40	0.0773	3.94
50	0.0993	5.06

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr 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) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1,3,5-cycloheptatriene in water at 25°C was reported to be 620 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0620 g(1)/100 g sln and 1.21 x 10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 20 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2] (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 p.
VARIABLES:	**PREPARED BY:**
Temperature: 278.26-318.36 K	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 1,3,5-cycloheptatriene in water

T/ K	g(1)/100 g sln	$10^3 x_1$
278.26	0.05809 ± 0.0014	0.1136
288.36	0.06645 ± 0.0017	0.1299
298.26	0.06694 ± 0.0019	0.1309
308.36	0.07418 ± 0.0019	0.1450
318.36	0.07648 ± 0.0022	0.1495

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) Columbia Organic Chemicals Co., Inc.; Tech 83%; used as received.

(2) laboratory distilled water.

ESTIMATED ERROR:

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

REFERENCES: