

COMPONENTS:	EVALUATOR:
(1) 1,4-Cyclohexadiene; C ₆ H ₈ ; [628-41-1]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia.
(2) Water; H ₂ O; [7732-18-5]	November 1984.

CRITICAL EVALUATION:

Quantitative data for the solubility of 1,4-cyclohexadiene (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of
1,4-Cyclohexadiene (1) in Water (2)

Reference	T/K	Method
McAuliffe (ref 1)	298	GLC
Pierotti and Liabastre (ref 2)	278-318	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. No data appear to have been reported for the solubility of water in 1,4-cyclohexadiene.

The solubility values of (1) in (2) are listed in Table 2. The data are in poor agreement, with those of Pierotti and Liabastre (ref 2) being approximately 20% (relative) higher than those of McAuliffe (ref 1). This situation is typical for a large number of hydrocarbon-water systems investigated by these authors and is discussed in greater detail in the Critical Evaluation of the cyclopentane-water system. In general the values of McAuliffe are much closer to accepted values (in well-characterised systems) than those of Pierotti and Liabastre. However, in the absence of confirmatory studies, the data of Pierotti and Liabastre are not rejected although they should probably be regarded only as order-of-magnitude values. The datum of McAuliffe may be considered as "Tentative".

TABLE 2: Solubility Values of 1,4-Cyclohexadiene (1) in Water (2)

T/K	Solubility values		
	Reported values ^a g(1)/100g sln	"Best" value ($\pm \sigma_n$) ^b g(1)/100g sln	$10^4 x_1$
278	0.085* (ref 2)	0.09	1.9
288	0.094* (ref 2)	0.09	2.1
298	0.070 (ref 1), 0.093*(ref 2)	0.08 \pm 0.01	2.1
308	0.09* (ref 2)	0.1	2.2
318	0.101 (ref 2)	0.1	2.3

Note: Footnotes to Table 2 on next page.

(continued next page)

<p>COMPONENTS:</p> <p>(1) 1,4-Cyclohexadiene; C₆H₈; [628-41-1]</p> <p>(2) Water; H₂O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia. November 1984.</p>
<p>CRITICAL EVALUATION: (continued)</p> <p><u>TABLE 2</u> (continued)</p> <p>a Values marked with asterisk (*) obtained by Evaluator by graphical interpolation of original measurements.</p> <p>b See comments in text regarding reliability of "Best" values; σ_n has no statistical significance.</p> <p>REFERENCES</p> <ol style="list-style-type: none">1. McAuliffe, C. <i>J. Phys. Chem.</i> <u>1966</u>, <i>70</i>, 1267-75.2. Pierotti, R.A.; Liabastre, A.A. <i>Structure and properties of water solutions</i>. U.S. Nat. Tech. Inform. Serv., PB Rep. <u>1972</u>, No. 21163, 113 pp.	

COMPONENTS: (1) 1,4-Cyclohexadiene; C ₆ H ₈ ; [628-41-1] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: McAuliffe, C. <i>J. Phys. Chem.</i> <u>1966</u> , 70, 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES: <p>The solubility of 1,4-cyclohexadiene in water at 25°C was reported to be 700 g(1)/10⁶ g(2).</p> <p>The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0700 g(1)/100 g sln and 1.57×10^{-4}.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>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.</p>	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5 K soly. 16 g(1)/10 ⁶ g(2) (standard deviation of mean) REFERENCES:

COMPONENTS: (1) 1,4-Cyclohexadiene; C ₆ H ₈ ; [628-41-1] (2) Water; H ₂ O; [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., <u>1972</u> , No. 21163, 113 p.																		
VARIABLES: Temperature: 278.26-318.36 K	PREPARED BY: M.C. Haulait-Pirson																		
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of 1,4-cyclohexadiene in water</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;"><u>T/K</u></th> <th style="text-align: center;"><u>g(1)/100 g sln</u></th> <th style="text-align: center;"><u>10³x₁</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">278.26</td> <td style="text-align: center;">0.08519 ± 0.0019</td> <td style="text-align: center;">0.1915</td> </tr> <tr> <td style="text-align: center;">288.36</td> <td style="text-align: center;">0.09585 ± 0.0028</td> <td style="text-align: center;">0.2155</td> </tr> <tr> <td style="text-align: center;">298.26</td> <td style="text-align: center;">0.09362 ± 0.0023</td> <td style="text-align: center;">0.2105</td> </tr> <tr> <td style="text-align: center;">308.36</td> <td style="text-align: center;">0.09634 ± 0.0023</td> <td style="text-align: center;">0.2166</td> </tr> <tr> <td style="text-align: center;">318.36</td> <td style="text-align: center;">0.10100 ± 0.0023</td> <td style="text-align: center;">0.2271</td> </tr> </tbody> </table>		<u>T/K</u>	<u>g(1)/100 g sln</u>	<u>10³x₁</u>	278.26	0.08519 ± 0.0019	0.1915	288.36	0.09585 ± 0.0028	0.2155	298.26	0.09362 ± 0.0023	0.2105	308.36	0.09634 ± 0.0023	0.2166	318.36	0.10100 ± 0.0023	0.2271
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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.; 99%; used as received. (2) laboratory distilled water. ESTIMATED ERROR: soly.: standard deviation from at least 15 measurements are given above. REFERENCES:																		