COMPONENTS:	EVALUATOR:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986

CRITICAL EVALUATION:

Quantitative solubility data for the tetradecane (1) - water (2) system have been reported in the publications listed in Table 1.

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

Reference	T /K	Solubility	Method
Schatzberg (ref 1)	313	(2) in (1)	Karl Fischer
Franks (ref 2)	298	(1) in (2)	GLC
Sutton and Calder (ref 3)	298	(1) in (2)	GLC
Mackay *et al.* (ref 4)	- [a]	(1) in (2)	GLC

a Not specified but probably close to 298 K.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF TETRADECANE (1) IN WATER (2)

The solubility of tetradecane in water has been reported only at 298K (Table 1). Unfortunately, the results are in very poor agreement (Table 2). Furthermore, all the reported values are very much higher than the value of ~ 3×10^{-8} g(1)/100 g sln which is predicted by extrapolation of the lower hydrocarbon homologue solubilities. Thus, the values given in Table 2 must be regarded very sceptically and no "Best" value has been calculated.

TABLE 2: Reported Solubility Values of Tetradecane (1) in Water (2)

T/K	Reported solubility values [a] 10^7 g(1)/100 g sln
298	6.94 (ref 2), 2.2 (ref 3), 25.9 [b] (ref 4)

a All values may be high. "Best" values not determined because of uncertainties in data, see text.

b Assumed to be at 298K for the purpose of comparison.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN TETRADECANE

As only the datum of Schatzberg at 313K is available no Critical Evaluation is possible. However, it may be noted that the data of Schatzberg in well characterized systems are generally reliable. The interested user is referred to the appropriate Data Sheet for the experimental value.

REFERENCES

1. Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.

2. Franks, F. *Nature (London)* 1966, *210*, 87-8.

3. Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8* , 654-7.

4. Mackay, D.; Shiu, W.J.; Wolkoff, A.W. "Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. 1975, *573* , 251-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.
VARIABLES:	**PREPARED BY:**
One temperature: 40°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in tetradecane at 40°C was reported to be 114 mg(2)/kg sln corresponding to a mole fraction, x_2, of 1.26×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade; 99+ mole %; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.02°C
soly. 0-2% (deviations from the mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Tetradecane; $H_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	Franks, F. *Nature (London)* 1966, *210*, 87-8.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	F. Kapuku

EXPERIMENTAL VALUES:

The solubility of tetradecane in water at 25°C was reported to be in mole fraction $x_1 = 6.3 \times 10^{-10}$.
The corresponding mass percent calculated by the compiler is 6.94×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analysis was performed by gas liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 mL of the aqueous phase was injected into the fractionator fitted to the chromatographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations.	(1) Fluka; purum grade; purity > 97% (chromatographic analysis). (2) not specified.
	ESTIMATED ERROR: soly. ± 12%
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of tetradecane in water at 25°C was reported to be 2.2×10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1, of 2×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
175 mg (1) were equilibrated with 700 mL (2) in closed flasks by shaking on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 μm Millipore filter, then extracted three times with 10-mL portions of hexane containing an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization detectors.	(1) Analabs Inc., 99+%. (2) doubly distilled.
	ESTIMATED ERROR: temp. ± 0.1°C soly. ± 16%
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.J.; Wolkoff, A.W. "Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. 1975, *573*, 251-8.
VARIABLES:	**PREPARED BY:**
not specified	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported a value of 0.0259 mg(1)dm^{-3} sln for the solubility of tetradecane in water.
With the assumption of a solution density of 1.00 g cm^{-3} the corresponding mass percent, calculated by the compiler, is 2.59×10^{-6} g(1)/100 g sln and the corresponding mole fraction, x_1, is 2.4×10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) is partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to the column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equilibrations it is possible to calculate the amount of (1) in the original sample.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not estimated.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Seawater	Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.
VARIABLES: One temperature: 25°C One salinity: 35 g salts/kg sln	**PREPARED BY:** P.A. Meyers and D. Shaw

EXPERIMENTAL VALUES:

The solubility of tetradecane in seawater was reported to be 1.7×10^{-7} g(1)/100 g sln and $x_1 = 1.5 \times 10^{-10}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 hrs at 25.0 ± 0.1°C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons.

Seawater collected from 25 m depth in Gulf of Mexico, poisoned with $HgCl_2$ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural n-alkane levels too low to cause interference.

ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental error of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

REFERENCES: