COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

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

April 1986.

CRITICAL EVALUATION:

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

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

Reference	*T*/K	Solubility	Method
Schatzberg (ref 1)	298,313	(2) in (1)	Karl Fischer
Franks (ref 2)	298	(1) in (2)	GLC
Sutton and Calder (ref 3)	298	(1) in (2)	GLC

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 DODECANE (1) IN WATER (2)

The solubility of dodecane in water has been reported in only two publications, both at 298K (Table 1). The agreement between the two studies is very poor with Franks value (ref 2) considerably higher than that reported by Sutton and Calder (ref 3). Support for the lower value comes from extrapolation of the lower *n*-alkane solubilities. However, there is sufficient uncertainty in this extrapolation to preclude rejection of the higher value at this time. The available data are summarized in Table 2.

TABLE 2: Tentative Solubility Values of Dodecane (1) in Water (2)

T/K	Solubility values		
	Reported values $10^7 g(1)/100g$ sln	"Best" value[a] $10^7 g(1)/100g$ sln	$10^{10}\ x_1$
298	8.42 (ref 2), 3.7 (ref 3)	3.7	3.9

a Datum from ref 3 preferred as Tentative value; see text.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Dodecane; $C_{12}H_{26}$; [112-40-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. April 1986.

CRITICAL EVALUATION: (continued)

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

As only the data of Schatzberg (ref 1) are available no Critical Evaluation is possible. However, it may be noted that the values of Schatzberg in well characterized systems are generally reliable. The interested user is referred to the relevant Data Sheet for the experimental values.

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.

COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Schatzberg, P.

J. Phys. Chem. 1963, *67*, 776-9.

VARIABLES:

Temperature: 25-40°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in dodecane

t/°C	mg(2)/kg sln	x_2
25	65[a]	6.1×10^{-4}
40	127[b]	12.0×10^{-4}

[a] See "Estimated Error"

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. a) 0-6%; b) 0-2% (deviations from the mean)

REFERENCES:

COMPONENTS: (1) Dodecane; $C_{12}H_{26}$; [112-40-3] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Franks, F. *Nature (London)* 1966, *210*, 87-8.
VARIABLES: One temperature: 25°C	**PREPARED BY:** F. Kapuku

EXPERIMENTAL VALUES:

The solubility of dodecane in water at 25°C was reported to be in mole fraction $x_1 = 8.9 \times 10^{-10}$.
The corresponding mass percent calculated by the compiler is 8.42×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka; purum grade; purity > 97% (chromatographic analysis).

(2) not specified.

ESTIMATED ERROR:

soly. ± 12%

REFERENCES:

COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

Environ. Sci. Technol. 1974, *8*, 654-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of dodecane in water at 25°C was reported to be 3.7×10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1 of 4×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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.

SOURCE AND PURITY OF MATERIALS:

(1) Analabs Inc., 99+%.

(2) doubly distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. ± 16%

REFERENCES:

COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

(2) Seawater

EVALUATOR:

D.G. Shaw
Institute of Marine Science
University of Alaska
Fairbanks, Alaska USA

December 1982

CRITICAL EVALUATION:

The solubility of dodecane (1) in seawater (2) at 298 K has been reported in three works:

Authors	Method	Salinity g salts/kg sln	10^7 g(1)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC	6	5
Sutton and Calder (ref 2)	GLC	35	2.9
Button (ref 3)	isotopic	12	1.74

The reported data are all from different salinities which precludes direct comparison. Since the data are in only fair agreement with each other and with the reported values for the solubility of dodecane in pure water, all three values are adopted as tentative.

SOLUBILITY OF DODECANE (1) IN SEAWATER (2)
TENTATIVE VALUE

T/K	g salts/kg sln	g(1)/100 g sln
298	35	2.9×10^{-7}

REFERENCES

1. Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Neftekhimiya*, 1973, *13*, 885-8.

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

3. Button, D.K. *Geochim. Cosmochim. Acta* 1975, *40*, 435-40.

COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

(2) Seawater

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.;
Gubergrits, M.Ya.

Neftekhimiya 1973, *13*, 885-8.

VARIABLES:

One temperature: 25°C
Salinity: 6 g/kg sln

PREPARED BY:

M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of dodecane in seawater was reported to be 5×10^{-7} g(1)/100 g sln. and the corresponding mole fraction, $x_1 = 5.0 \times 10^{-10}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

SOURCE AND PURITY OF MATERIALS:

(1) "chemically pure"

(2) distilled water plus salt mixture.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

(2) Seawater

ORIGINAL MEASUREMENTS:

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 dodecane in seawater was reported to be 2.9×10^{-7} g(1)/100 g sln and $x_1 = 3.1 \times 10^{-10}$.

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:

COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

(2) Salt mixture (ref 1)

(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Button, D. K.

Geochim. Cosmochim. Acta 1975,
40, 435-40.

VARIABLES:

One temperature: 25°C
Constant salinity: 12 g(2)/kg sln
Different periods of standing

PREPARED BY:

P. Meyers and D. Shaw

EXPERIMENTAL VALUES:

Dodecene concentration in saline medium after gently stirring for 1 week and then remaining quiescent for the periods shown

Time, Weeks	Dodecane, μg(1)/L(2)
1	2.16 ± 0.03
8	1.80 ± 0.02
16	1.78 ± 0.02

The corresponding mass percent and mole fraction calculated by the compilers for the results at 16 weeks are 1.74 x 10^{-7} g(1)/100 g sln and 1.89 x 10^{-10} using the assumption that the solution density is 1.02 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Dodecane solutions were prepared in a chemically defined solution resembling dilute seawater. In addition to the mineral salts and vitamins reported (ref 1), the solution contained 1 mg/L arginine and 10 g/L NaCl. After sterilization (121°C for 30 min), 0·8 μL of ^{14}C-dodecane was sprayed on to the medium surface to form a thin film. Gentle subsurface agitation was induced by a 3 in magnet rotating at 60 rev/min against the inside carboy wall at midlevel. The subsurface dodecane concentration was determined from the radioactivity of samples collected from a port at the bottom of the carboy. The system was stirred for 1 week and then allowed to stand. Equilibrium appeared to have been achieved within 8 weeks.

SOURCE AND PURITY OF MATERIALS:

Amersham Searle Corp. (Arlington Heights, Ill.) supplied the [1-^{14}C] dodecane, 27 μCi/μmol. It was accompanied by a gas chromatogram of the preparation showing a single peak at the appropriate location.

ESTIMATED ERROR:

Experimental error is estimated at ± 1%.

REFERENCES:

1. Button, D. K. *Limnol. Oceanogr.* 1969, *14*, 95-100.