COMPONENTS:	EVALUATOR:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1984.

CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Führer (ref 1)	289	(1) in (2)	titration
Black *et al.* (ref 3)	279-298	(2) in (1)	radiotracer
Namiot and Beider (ref 4)	293-345[a]	(1) in (2)	gas-liq. equilibrium
Wishnia (ref 5)	263-308	(1) in (2)	radiotracer
Barone *et al.* (ref 6)	298	(1) in (2)	GLC
Connolly (ref 7)	573-625[a]	(1) in (2)	cloud point
McAuliffe (ref 8)	298	(1) in (2)	GLC
Nelson and DeLigny (ref 9)	277-303	(1) in (2)	GLC
Pierotti and Liabastre (ref 10)	278-308	(1) in (2)	GLC
Polak and Lu (ref 11)	273,298	mutual	GLC, Karl Fischer
Price (ref 13)	298-423	(1) in (2)	GLC
Korenman and Aref'eva (ref 14)	293	(1) in (2)	titration
Krzyzanowska and Szeliga (ref 15)	298	(1) in (2)	GLC
Rudakov and Lutsyk (ref 16)	298	(1) in (2)	partition coefficient
Jonsson *et al.* (ref 17)	288-308	(1) in (2)	partition coefficient

[a]Pressure also varied.

Solubility data for pentane in water may also be calculated from the calorimetric data of Gill *et al.* (ref 12). Apart from the work of Scheffer (ref 2) and Roof (ref 18) which did not contain sufficient information to justify inclusion, and Wishnia (ref 5) who reported only graphical information, all the original measurements in the references listed in Table 1 are compiled in the Data Sheets immediately following this Critical Evaluation.

As indicated in the footnote to Table 1, quantitative solubility data for pentane in water at elevated pressures have been reported in the papers by Namiot and Beider (ref 4) and Connolly (ref 7). Since these studies were not carried out under comparable conditions no critical evaluation of their reliability can be made and the interested user is referred to the original measurements in the relevant Data Sheets. Connolly (ref 7) reports an upper critical solution temperature of 624K at 34 MPa whilst Roof (ref 18) reports a three phase critical equilibrium point at 464K and 658 psia (4.5 MPa).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Pentane; C_5H_{12}; [109-66-0]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1984.
(2) Water; H_2O; [7732-18-5]	

CRITICAL EVALUATION: (continued)

In the Tables which follow, solubilities obtained by the Evaluator by graphical interpolation of the original measurements in the Data Sheets are indicated by an asterisk (*). "Best" values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than as error limits.

For convenience, further discussion of the solubility data for this system will be divided into two parts.

1. THE SOLUBILITY OF PENTANE (1) IN WATER (2)

Only five studies (ref 9, 10, 11, 13, 17) report the solubility of pentane in water as a function of temperature. The data of Nelson and DeLigny (ref 9), Polak and Lu (ref 11), Price (ref 12) and Jonsson *et al.* (ref 17) are in good agreement with each other given the analytical difficulties at the low concentrations involved. However, the solubilities of Pierotti and Liabastre (ref 10) are approximately twice as high as the other studies (ref 9, 11, 13, 17). Since Pierotti and Liabastre's data are also markedly higher than all other values at 298K (ref 6, 8, 9, 11, 13, 16, 17) and are generally higher than "Recommended" values for well-characterized systems (e.g. benzene in water), their results are rejected.

The data of Fühner (ref 1) at 298K and Korenman and Aref'eva (ref 14) at 293K are also markedly higher than all other values and are therefore rejected. The data of Krzyzanowska and Szeliga (ref 15) do not appear to be independent of those of Price (ref 13) and have therefore been excluded from this Critical Evaluation. All other data are included in Table 2.

TABLE 2: Recommended (*R*) and Tentative Values of the Solubility of Pentane (1) in Water (2)

T/K	Solubility values		
	Reported values 10^3g(1)/100g sln	"Best" values ($\pm \sigma_n$) 10^3g(1)/100g sln	$10^5 x_1$
273	6.57 (ref 11)	6.6	1.7
283	4.29 (ref 9)	4.3	1.1
293	3.93 (ref 9), 4.14 (ref 17)	4.0 ± 0.1 (*R*)	1.0(*R*)
298	4.97 (ref 6), 3.85 (ref 8), 4.05 (ref 9), 4.76 (ref 11), 3.95 (ref 13), 4.06 (ref 16), 4.06 (ref 17)	4.2 ± 0.4	1.1

(Table 2 continued next page)

COMPONENTS:	EVALUATOR:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1984.

CRITICAL EVALUATION: (continued)

TABLE 2 (continued)

T/K	Solubility values		
	Reported values $10^3 g(1)/100g$ sln	"Best" values ($\pm \sigma_n$) $10^3 g(1)/100g$ sln	$10^5 x_1$
303	4.05 (ref 9), 4.1 (ref 13), 4.03 (ref 17)	4.1 ± 0.1 (*R*)	1.0 (*R*)
313	3.98* (ref 13)	4.0	1.0
323	4.1* (ref 13)	4.1	1.0
333	4.3* (ref 13)	4.3	1.1
343	4.6* (ref 13)	4.6	1.2
353	5.0* (ref 13)	5.0	1.3
363	5.8* (ref 13)	5.8	1.5
383	8.6* (ref 13)	8.6	2.2
403	15.0* (ref 13)	15	3.8
423	30.3* (ref 13)	30	7.5

As is obvious from Table 2, the solubilities at temperatures other than 298K are mainly those of Price (ref 13) and in the absence of confirmatory studies can only be regarded as tentative. However, the agreement with other studies at 298K, as noted above, is quite good and, furthermore, application of the van't Hoff equation to the data listed in Table 2 gives ΔH^{∞}_{sln} = -4.72 kJ mol^{-1} and $\Delta C^{\infty}_{p,sln}$ = 379 JK^{-1} mol^{-1} which agree well with the calorimetrically determined values (ref 12) of -2.0 ± 0.2 kJ mol^{-1} and 400 ± 70 JK^{-1} mol^{-1}. Thus some confidence can be placed in the "best" values. Selected data are plotted in Figure 1.

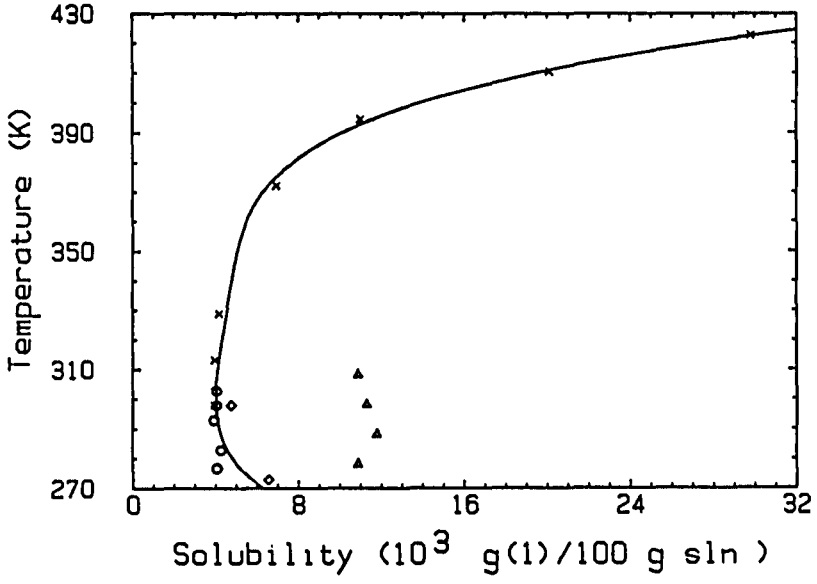

FIGURE 1. Solubility of pentane in water: ref 13 (x); ref 9 (o); ref 11 (◇); ref 10 (△, rejected data, see text). (cont'nued)

COMPONENTS:	EVALUATOR:
(1) Pentane; C_5H_{12}; [109-66-0]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H_2O; [7732-18-5]	October 1984.

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN PENTANE (1)

The solubility of water in pentane has been reported only by Black *et al.* (ref 3) and Polak and Lu (ref 11). Their results are mutually consistent but in the absence of confirmatory data they must be considered as "Tentative" only. The data are listed in Table 3 and plotted in Figure 2.

TABLE 3: Tentative Values of the Solubility of Water (2) in Pentane (1)

T/K	Solubility values		
	Reported values $10^3 g(2)/100g$ sln	"Best" values ($\pm \sigma_n$) $10^3 g(2)/100g$ sln	$10^5 x_2$
273	2.6 (ref 11)		
283	4.2* (ref 3)		
293	8.5* (ref 3		
298	12.2* (ref 3), 10.1 (ref 11)	11 ± 1	4.4

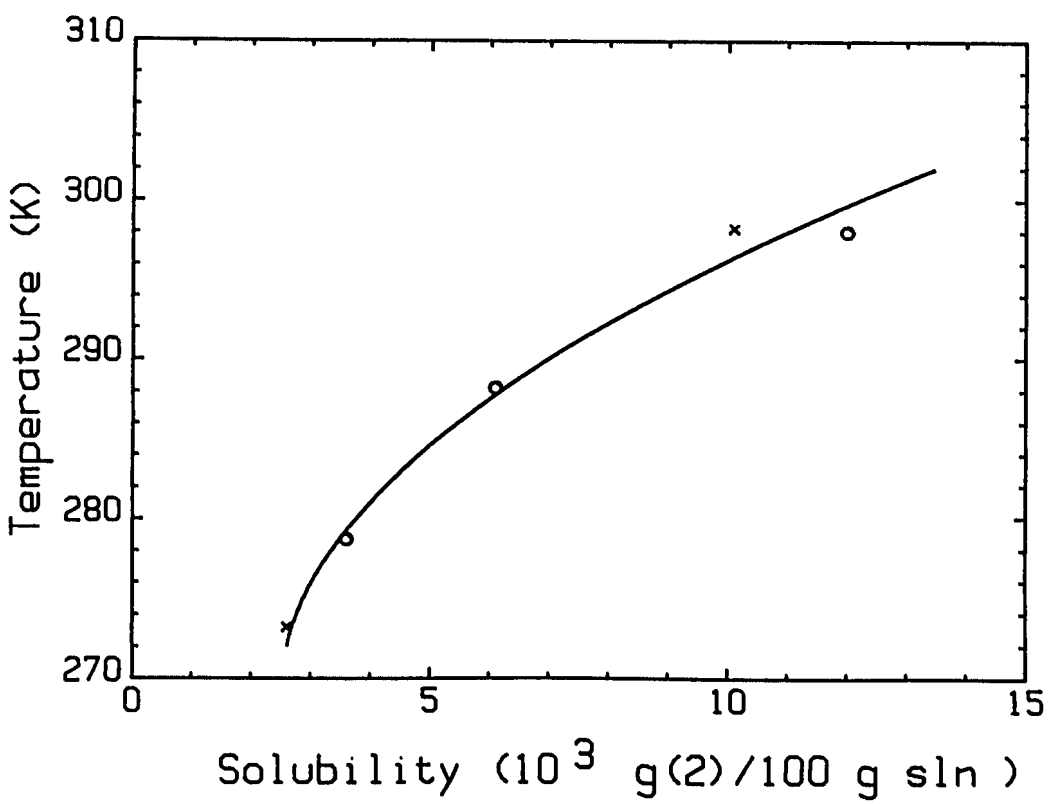

FIGURE 2. Solubility of water in pentane: ref 3 (o); ref 11 (x). (continued)

COMPONENTS:	EVALUATOR:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1984.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Fühner, H. *Chem. Ber.* 1924, *57*, 510-15.
2. Scheffer, F.E.C. *Proc. Roy. Acad. Amsterdam* 1914, *17* , 834.
3. Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* 1948, *16* , 537-43.
4. Namiot, A.Yu.; Beider, S.Ya. *Khim. Tekhnol. Topl. Masel* 1960, *7* , 52-5.
5. Wishnia, A. *J. Phys. Chem.* 1963, *67* , 2079.
6. Barone, G.; Crescenzi, V.; Pispisa, B.; Quadrifoglio, F. *J. Macromol. Chem.* 1966, *1* , 761-71.
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15. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.
16. Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* 1979, *53* , 1298-1300.
17. Jonsson, J.A.; Vejrosta, J.; Novak, J. *Fluid Phase Equil.* 1982, *9* , 279-86.
18. Roof, J.G. *J. Chem. Eng. Data* 1970, *15*, 301-3.

ACKNOWLEDGEMENTS

The evaluator thanks Dr Brian Clare for the regression analyses and Dr Marie-Claire Haulait-Pirson for comments.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Führer, H. *Ber. Dtsch. Chem. Ges.* 1924, *57*, 510-15.
VARIABLES:	**PREPARED BY:**
One temperature: 16°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of pentane in water at 16°C was reported to be 0.060 mL (1)/100 mL sln or 0.036 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compiler is 9.0×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a stoppered measuring cylinder pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100 or 1000 cm^3 of (2) until a completely clear solution was obtained at the experimental temperature.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; commercial grade; used as received.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0]	Black, C.; Joris, G.G.; Taylor, H.S.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Phys.* 1948, *16*, 537-43.
VARIABLES:	**PREPARED BY:**
Temperature: 5.5-24.8°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in pentane
at a total saturation pressure of 1 atm

t/°C	g(2)/100 g(1)	g(2)/100 g sln (compiler)	$10^4 x_2$ (compiler)
5.5	0.0036	0.0036	1.44
15.0	0.0061	0.0061	2.45
24.8	0.0119	0.0119	4.77
24.8	0.0120	0.0120	4.81

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method described in ref 1 in which tritium oxide acts as a tracer, was used.
Air saturated with radioactive water vapor was bubbled through the (1) sample until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred in the counter through equilibration with ethanol vapor.

SOURCE AND PURITY OF MATERIALS:

(1) Ohio State University under an American Petroleum Institute project; purity not specified; used as received.

(2) not specified.

ESTIMATED ERROR:

soly. a few percent (type of error not specified).

REFERENCES:

1. Joris, G.G.; Taylor, H.S.
J. Chem. Phys. 1948, *16*, 45.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Namiot, A. Yu; Bender, S. Ya. *Khim. Tekhnol. Topl. Masel* 1960, *7*, 52-5.
VARIABLES:	**PREPARED BY:**
Temperature: 20-71.4°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of pentane in water at 32 atm.

t/°C	g(1)/100 g sln	$10^5 x_1$
20	0.011	2.7
37.8	0.015	3.9
71.4	0.026	6.4

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined from gas-liquid equilibrium measurements in the ternary system pentane-water-methane at 32 atm. in an apparatus described in ref 1.

No more details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Rogov, B.A.; Namiot, A. Yu.; Bondareva, M.M. *Tr. Vses. Neftegazov. Nauch. Issled. Inst.* 1958, *15*, 196.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Barone, G.; Crescenzi, V.; Pispisa, B.; Quadrifoglio, F. *J. Macromol. Chem.* 1966, *1*, 761-71.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors report a value of 0.00103 mol(1)/dm^3(2) for the solubility of pentane in water at 25°C. This value is the experimental one multiplied by 760/p where p is the partial pressure of (1) over (2). p = 508 mm Hg. The solubility at system pressure calculated by the compiler is 6.88 x 10^{-4} mol(1)/dm^3(2) and the corresponding mass percent and mole fraction, x_1, are 0.00497 g(1)/100 g sln and 1.24 x 10^{-5} (with the assumption of a solution density of 1 g cm^{-3}).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturation was carried out by bubbling the vaporized (1) into the solution and letting an excess of the condensed (1) stand in contact with the aqueous phase for more than 12 hr at 25°C under gentle shaking. 0.20 mL samples of (2) saturated with (1) were taken with a calibrated syringe and injected into the chromatographic column packed with 15% of poly(propylene glycol) on chromosorb. A gas chromatography unit having a tungsten-wire katharometer as detector was employed. More details are given in the paper.	(1) RP product, C. Erba, Milan; chromatographically pure. (2) not specified.
	ESTIMATED ERROR: temp. ± 0.02 K soly. ± 4% (type of error not specified).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0]	Connolly, J.F.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Eng. Data* 1966, *11*, 13-6.
VARIABLES:	**PREPARED BY:**
Temperature: 300-325°C Pressure: 150-700 atm	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of pentane in water

t/°C	p/atm	p/MPa (compiler)	g(1)100 g sln	x_1 (compiler)
300	150	15.2	1.3	0.0033
	185	18.7	1.7	0.0043
	350	35.4	1.7	0.0043
	600	60.7	1.6	0.0040
	700	70.9	1.5	0.0038
330	170	17.2	2.1	0.0053
	195	19.7	3.3	0.0084
	220	22.2	4.0	0.0103
	260	26.3	4.6	0.0119
	350	35.4	4.9	0.0127
	485	49.1	4.7	0.0122
	670	67.8	4.0	0.0103
340	230	23.3	5.2	0.0135
	250	25.3	6.1	0.0160
	275	27.8	6.9	0.0182
	330	33.4	7.6	0.0201
	350	35.4	7.6	0.0201
	470	47.6	6.9	0.0182
	620	62.8	5.7	0.0149

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The cloud point method was used. Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected, until either a cloud or a small portion of a second phase appeared at the top of the cell. Then mercury was injected to change the pressure, more (1) was injected and the procedure was repeated.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips reagent grade; better than 99.8%; used as received.

(2) distilled and deaerated.

ESTIMATED ERROR:

temp. ± 0.02 K
press. ± 2 atm (accuracy)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0]	Connolly, J.F.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Eng. Data* 1966, *11*, 13-6.

t/°C	p/atm	p/MPa (compiler)	g(1)100 g sln	$x1$ (compiler)
350	240	24.31	7.8	0.0207
	225	25.83	9.0	0.0241
	265	26.84	10.3	0.0279
	280	28.36	12.1	0.0332
	300	30.39	13.9	0.0387
	325	32.92	15.5	0.0438
	350	35.46	15.5	0.0438
	395	40.01	13.9	0.0387
	445	45.08	12.0	0.0329
	510	51.66	10.3	0.0279
	590	59.77	9.0	0.0241
352	280	28.36	15.8	0.0442
	280	28.36	18.4	0.0533
	280	28.36	21.0	0.0622
	280	28.36	23.3	0.0705
	400	40.52	40.7	0.1463
	390	39.51	38.7	0.1362
	385	39.00	36.5	0.1255
	380	38.49	34.0	0.1140
	375	37.99	31.4	0.1026
	375	37.99	28.5	0.0905
	375	37.99	25.4	0.0784
	375	37.99	23.3	0.0705
	380	38.49	21.0	0.0622
	390	39.51	18.4	0.0533
	420	42.55	15.7	0.0444

COMMENTS AND ADDITIONAL DATA:

Upper critical solution temperature: 351°C at p = 340 atm.

The uncertainty in the CST is about 2°C and that of the corresponding pressure about 10 atm.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of pentane in water at 25°C was reported to be 38.5 mg (1)/kg sln, (0.0385 g/100 g sln).
The corresponding mole fraction, x_1, calculated by the compiler, is 9.6×10^{-6}.
The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250 mL glass 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. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 µL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+% purity; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5 K
soly. 2 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

1. McAuliffe, C. *Nature (London)* 1963, *200*, 1092.
2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* 1964, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Nelson, H.D.; De Ligny, C.L. *Rec. Trav. Chim. Pays-Bas* 1968, *87*, 528-44.
VARIABLES:	**PREPARED BY:**
Temperature: 4-30°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of pentane in water

t/°C	$10^5 x_1$	mg(1)/kg sln (compiler)
4.0	1.02 ± 0.20	40.9
10.0	1.07 ± 0.15	42.9
20.0	0.98 ± 0.19	39.3
25.0	1.01 ± 0.12	40.5
30.0	1.01 ± 0.17	40.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturation vessel is drawn in the original paper. (2) was saturated with (1) via the vapor phase: a few drops of (1) were put on the bottom of a tight-fitting flask containing a small flask filled with water. Complete saturation was reached by shaking overnight in an upright position. Samples were taken from the aqueous solution with a microsyringe through the septum and injected into the gas chromatograph equipped with a flame ionization detector. The gas chromatographic conditions are described in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips pure grade.

(2) tap-water was refluxed for 8 hours in the presence of $KMnO_4$ and KOH and distilled. The whole process was repeated once more.

ESTIMATED ERROR:

soly.: error given above (90% probability interval)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (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 pp.
VARIABLES:	**PREPARED BY:**
Temperature: 278.26-308.36 K	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of pentane in water

T/ K	g(1)/100 g sln	$10^3 x_1$	g(1)/100 g sln (corrected by compiler)
278.26	0.001094 ± 0.000037	0.02732	0.01094
288.36	0.001180 ± 0.000034	0.02946	0.01180
298.26	0.001128 ± 0.000045	0.02816	0.01128
308.36	0.001089 ± 0.000051	0.02719	0.01089

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 a 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) Fisher Scientific Co.; certified grade; used as received.

(2) laboratory distilled water.

ESTIMATED ERROR:

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

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
VARIABLES:	**PREPARED BY:**
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of pentane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0[a]	65.7[c]	1.64×10^{-5}
25[b]	47.6[c]	1.19×10^{-5}

Solubility of water in pentane

t/°C	mg(2)/kg sln	x_2 (compiler)
0[a]	26[d]	1.04×10^{-4}
25[b]	101[e]	4.04×10^{-4}

[a-e]see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

temp. a) ± 0.02 K; b) ± 0.01 K
soly. c) ± 1.7%; d) ± 4.7%;
e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0]	Price, L.C.
(2) Water; H_2O; [7732-18-5]	*Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	**PREPARED BY:**
Temperature: 25-149.5°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of pentane in water at system pressure

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^5 x_1$ (compiler)
25.0	39.5 ± 0.6	0.00395	0.99
40.1	39.8 ± 0.9	0.00398	0.99
55.7	41.8 ± 1.3	0.00418	1.04
99.1	69.4 ± 1.1	0.00694	1.73
121.3	110.0 ± 10.0	0.0110	2.74
137.3	201.0 ± 5.0	0.0201	5.01
149.5	298.0 ± 14.0	0.0298	7.43

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Room-temperature solubilities were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and ensured saturation (in 2 to 4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of the gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1 K
soly. range of values given above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Korenman, I.M.; Aref'eva, R.P. Patent USSR, 553 524, 1977.04.05 C.A. *87*:87654
VARIABLES: One temperature: 20°C	**PREPARED BY:** A. Maczynski

EXPERIMENTAL VALUES:

The solubility of pentane in water at 20°C was reported to be 0.7 g(1)dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.07 g(1)/100 g sln and 1.7×10^{-4}. The assumption that 1 dm^3 sln = 1 kg sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
About 100-500 mL(2) was placed in a glass cylinder and 10-50 mg of an insoluble indicator was added and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall 2-3 cm above the liquid layer. After each drop of (1), the mixture was vigorously mixed for 0.5-1.5 min.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES: