COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION:

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

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

Reference	*T*/K	Solubility	Method
Herz (ref 1)	295	(1) in (2)	densimetric
Fühner (ref 3)	289	(1) in (2)	titration
Milligan (ref 4)	298	(1) in (2)	partition coefficient
Bennett and Philip (ref 5)	290	(1) in (2)	volumetric
Booth and Everson (ref 6)	298	(1) in (2)	residue volume
Gester (ref 7)	298-328	(2) in (1)	Karl Fischer
Black *et al.* (ref 8)	293	(2) in (1)	radiotracer
Durand (ref 9)	289	(1) in (2)	cloud point
McBain and Lissant (ref 10)	298	(1) in (2)	cloud point
McCants *et al.* (ref 11,12)	311	mutual	cloud point
Kudchadker and McKetta (ref 13)	311-411^a	(1) in (2)	not specified
Englin *et al.* (ref 14)	293-313	(2) in (1)	analytical
Zel'venskii *et al.* (ref 15)	293	(2) in (1)	radiotracer
Barone *et al.* (ref 16)	298	(1) in (2)	GLC
McAuliffe (ref 17)	298	(1) in (2)	GLC
Burd and Braun (ref 18)	355-478^a	(2) in (1)	GLC
Nelson and DeLigny (ref 19)	277-328	(1) in (2)	GLC
Roddy and Coleman (ref 20)	298	(2) in (1)	GLC
Benkovski *et al.* (ref 21)	303	(2) in (1)	Karl Fischer
Krasnoshchekova and Gubergrits (ref 22)	298	(1) in (2)	GLC
Skripka *et al.* (ref 23, 28, 30)	473,493^a	(2) in (1)	vap.liq. equilibrium
Leinonen and MacKay (ref 24)	298	(1) in (2)	GLC
Polak and Lu (ref 25)	273,298	(1) in (2)	GLC
Mackay *et al.* (ref 26)	unspecified	(1) in (2)	GLC
Budantseva *et al.* (ref 27)	293	mutual	GLC
Price (ref 29)	298-425	(1) in (2)	GLC

(Table 1 continued next page)

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

TABLE 1 (continued)

Reference	T/K	Solubility	Method
Korenman and Aref'eva (ref 31,34)	293,298	(1) in (2)	titration
Sugi and Katayama (ref 32)	298	(2) in (1)	Karl Fischer
Charykov *et al.* (ref 33)	293	(2) in (1)	Karl Fischer
Krzyzanowska and Szeliga (ref 35)	298	(1) in (2)	GLC
Aquan-Yuen *et al.* (ref 36)	298	(1) in (2)	GLC
Jonsson *et al.* (ref 38)	288-308	(1) in (2)	GLC
De Loos *et al.* (ref 39)	610-675[a]	mutual	synthetic
Tsonopoulos and Wilson (ref 40)	313-422[a]	mutual	GLC, Karl Fischer
Rebert and Hayworth (ref 41)	493-645[a]	(1) in (2)	synthetic

[a] Also studied at variable pressure, see Table 4.

Apart from the following exceptions, original data in all the references listed in Table 1 are compiled in the Data Sheets immediately following this Critical Evaluation. The work of Herz (ref 1) and Milligan (ref 4) have not been compiled because they employed petroleum fractions of unspecified composition rather than pure hexane. The work of Scheffer and Roof (ref 2,42; critical point data only), Bennett and Philip (ref 5; order of magnitude solubility only) and Gester (ref 7; graphical data only) did not contain sufficient information to justify compilation. Solubility data for hexane in water may also be obtained from the calorimetric data of Gill *et al.* (ref 37).

Despite the relatively large number of studies of the hexane-water system (Table 1) little information is available on the temperature dependence of the mutual solubilities of hexane and water. Even when comparable data are available, independently obtained values often differ by an order of magnitude. This system warrants thorough re-investigation at all temperatures.

In the Tables which follow, values obtained by the Evaluator by graphical interpolation of the original measurements contained in the Data Sheets are indicated by an asterisk (*). "Best" values have been obtained by simple averaging. 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 reported values rather than as error limits.

For convenience, further discussion of this system will be divided into three parts.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

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

The various data reported for the solubility of hexane in water are in poor agreement.

The value of Mackay *et al.* (ref 26) is rejected because the temperature was not specified. The data of Krzyzanowska and Szeliga (ref 35) have been excluded from consideration as they do not appear to be independent of those of Price (ref 29).

Of the remaining data, the results of Führer (ref 3), Booth and Everson (ref 6, order of magnitude), Durand (ref 9), McBain and Lissant (ref 10), Kudchadker and McKetta (ref 13, atmospheric pressure data only), McCants *et al.* (ref 11,12) Barone *et al.* (ref 16), Nelson and De Ligny (ref 19) and Korenman and Aref'eva (ref 31,34) are markedly higher, sometimes by an order of magnitude, than other results and are therefore rejected. All other data are included in Table 2 on the next page.

At 298K, the temperature where there is a reasonable number of independent determinations (Table 2), the various values are in reasonable agreement although the uncertainty on the average result means that it can be considered as "Tentative" only. This is almost certainly a reflection of the difficulties of accurate analysis of the very low concentrations involved even when using modern techniques (it is interesting to note that all the data at 298K were obtained by GLC methods).

At other temperatures, the results of Price (ref 29) and Tsonopoulos and Wilson (ref 40) are in quite good agreement up to 353K but begin to diverge at higher temperatures (Table 2 and Figure 1). Application of the van't Hoff equation to a combination of both data sets (ref 29,40) yields values for ΔH^{∞}_{sln} = 1.87 kJ mol^{-1}, $\Delta C^{\infty}_{p,sln}$ = 296 JK^{-1} mol^{-1} which are in relatively poor agreement with the calorimetric values of ΔH^{∞}_{sln} = 0.0 ± 0.2 kJ mol^{-1} and $\Delta C^{\infty}_{p,sln}$ = 440 ± 45 JK^{-1} mol^{-1} reported by Gill *et al.* (ref 37). In view of the disparities at higher temperatures, the uncertainty in the 298K value, and the poor agreement with calorimetric data, none of averaged "Best" values have been Recommended.

Figure 1 plots a selection of the solubility data of hexane in water. As well as the values of Price (ref 29) and Tsonopoulos and Wilson (ref 40), referred to above, the rejected data of Nelson and De Ligny (ref 19) have also been included for comparison.

(continued next page)

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

EVALUATOR:

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

October 1986.

CRITICAL EVALUATION: (continued)

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

T/K	Solubility values		
	Reported values	"Best" values (± σ_n)[a]	
	10^3g(1)/100g sln	10^3g(1)/100g sln	$10^6 x_1$
273	1.65 (ref 25)	1.7	3.5
293	1.4 (ref 27), 1.03 (ref 38)	1.2 ± 0.2	2.5
298	0.95 (ref 17), 1.3 (ref 22), 1.2 (ref 24), 1.24 (ref 25) 0.95 (ref 29), 1.23 (ref 36) 1.01 (ref 38)	1.1 ± 0.1	2.3
303	0.97* (ref 29), 1.00 (ref 38)	0.99 ± 0.02	2.1
313	1.04* (ref 29), 1.15[b] (ref 40)	1.10 ± 0.06	2.3
323	1.17* (ref 29), 1.23[b] (ref 40)	1.20 ± 0.03	2.5
333	1.34* (ref 29), 1.38[b] (ref 40)	1.36 ± 0.02	2.8
343	1.54* (ref 29), 1.60[b] (ref 40)	1.57 ± 0.03	3.3
353	1.77* (ref 29), 1.93[b] (ref 40)	1.85 ± 0.08	3.9
373	2.28* (ref 29), 3.06[b] (ref 40)	2.7 ± 0.4	5.6
393	3.60* (ref 29), 5.36[b] (ref 40)	4.5 ± 0.9	9.4
413	6.5* (ref 29), 10.1[b] (ref 40)	8 ± 2	16

[a] No "Best" values Recommended because of uncertainties in data, see text.

[b] Calculated from the original authors' fitting equation over the range of their experimental data.

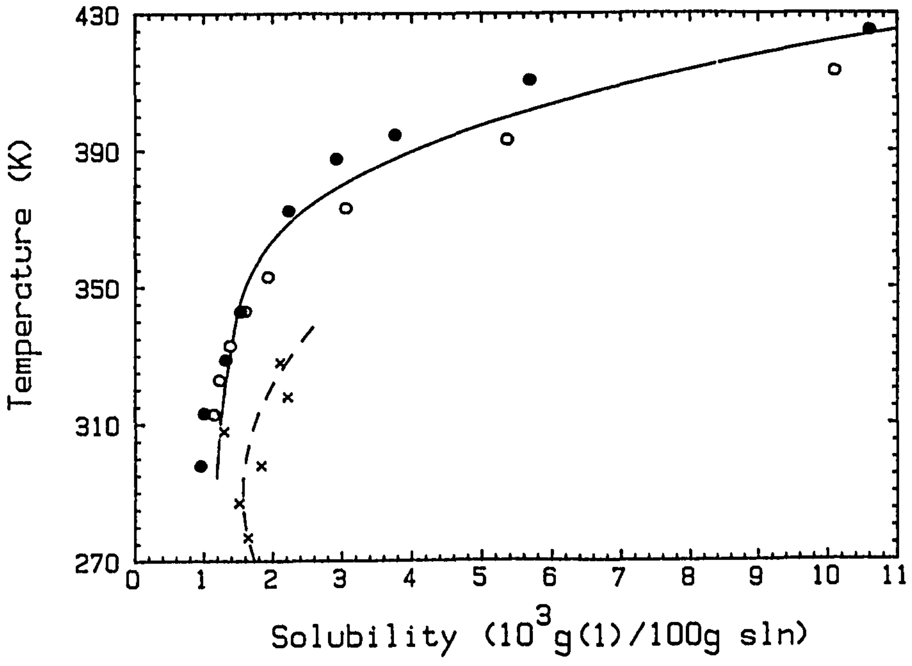

FIGURE 1. Solubility of hexane in water, selected data: ref 19 (x, rejected data); ref 29 (●); ref 40 (o).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

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

Solubility data for water in hexane are listed in Table 3, apart from the values of McCants *et al.* (ref 11,12), which are an order of magnitude higher than all other studies and have therefore been rejected.

In general, agreement amongst independently obtained values is poor (Table 3). This is probably a reflection of the difficulties of accurate analysis at these low concentrations. No data have been Recommended.

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

T/K	Solubility values		
	Reported values	"Best" values (± σ_n)	
	10^2g(1)/100g sln	10^2g(1)/100g sln	10^4x_2
273	1.01 (ref 14), 0.28 (ref 25)	0.6 ± 0.4	2.9
293	1.11 (ref 8), 1.66 (ref 15) 0.77 (ref 27), 0.836 (ref 33)	1.1 ± 0.4	5.3
298	0.995 (ref 20), 0.90 (ref 25), 1.07 (ref 32)	0.98 ± 0.07	4.7
303	1.79 (ref 14), 0.51 (ref 21)	1.1 ± 0.6	5.3
313	3.17 (ref 14), 2.51^a (ref 40)	2.8 ± 0.3	13
323	2.65^a (ref 40)	2.7	13
333	3.88^a (ref 40)	3.9	19
343	5.60^a (ref 40)	5.6	27
353	7.95^a (ref 40)	8.0	38

[a] Calculated from the original authors' fitting equation over the range of their experimental values.

Figure 2 plots all the available data for the solubility of water in hexane. The smooth curve which has been fitted to the "Best" values (Table 3) has the form s (10^2g(1)/100g sln) = 86.5345 - 0.6183 T + 0.00113 T^2 with R^2 = 0.977 and σ = 0.446, 293 ≤ T ≤ 353 K.

Application of the van't Hoff equation to the "Best" values gives ΔH^∞_{sln} = 28.7 kJ mol^{-1} and $\Delta C^\infty_{p,sln}$ = 73 JK^{-1} mol^{-1} for the dissolution of water in hexane. These values are broadly similar to those reported for other hydrocarbons and suggests, despite the lack of agreement amongst the individual studies in Table 3, that the Tentative "Best" values are reasonably reliable.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. October 1986.

CRITICAL EVALUATION: (continued)

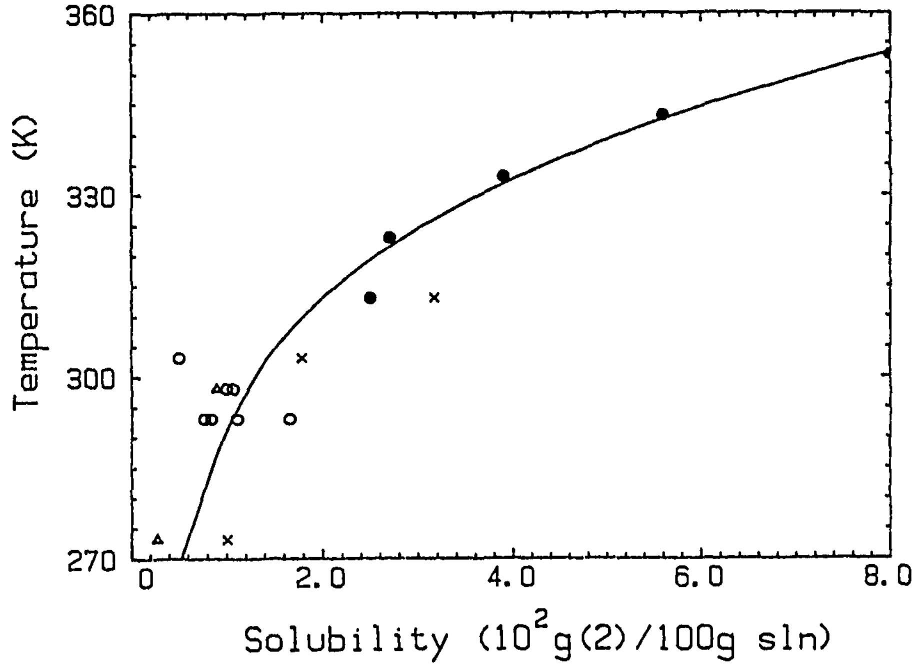

FIGURE 2. Solubility of water in hexane: ref 14 (x); ref 25 (Δ); ref 40 (●); other data (O). Line of best fit calculated for averaged "Best" values, see text.

3. MUTUAL SOLUBILITIES OF HEXANE (1) AND WATER (2) AT ELEVATED PRESSURES

This system exhibits the phenomenon of gas-gas immiscibility of the second kind and has type III phase behaviour (ref 43,44). In order to clarify the relationship between the phases in equilibrium it is convenient to consider the pressure-temperature projection of the pressure-temperature-composition diagram. A schematic representation of this projection for water + hexane is given in Figure 3. There are two critical lines, one starting at the critical point of hexane and ending on a three phase line. It should be noted that the three phase line on a pressure-temperature projection corresponds to three lines on the pressure-temperature-composition diagram, representing the composition of gas, liquid 1 and liquid 2 in equilibrium. The second critical line starts at the critical point of water, moves to lower temperatures at high pressures, passes through a minimum in temperature and eventually goes to temperatures greater than that of the critical point of water (this behaviour is referred to as gas-gas immiscibility of the second kind).

In the region above the three phase line on the p, T projection there is no vapor phase but may be a maximum of two liquid phases. Whether there is (are) one or two liquid phases depends on the overall composition. To the

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. October 1986.

CRITICAL EVALUATION: (continued)

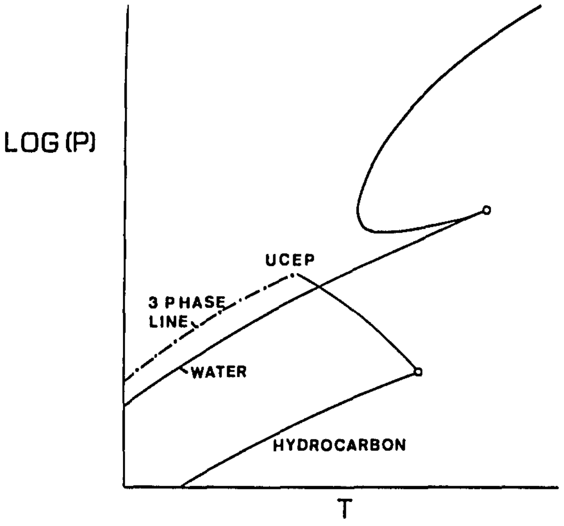

FIGURE 3: Pressure-temperature projection of the equilibrium-pressure-temperature-composition surface for the hexane-water system.

left of the critical line starting at the critical point of water it may be possible to have one or two phases present depending on the overall composition.

Solubility studies of the hexane-water system at pressures higher than atmospheric are listed in Table 4.

TABLE 4: Solubility Studies of the Hexane-Water System at Elevated Pressures

Reference	p/MPa	T/K	Solubility
Scheffer (ref 2)	5.274[b]	495.2[b]	-[b]
Kudchadker and McKetta (ref 13)	0.2 - 3.6	311-411	(1) in (2)
Burd and Braun (ref 18)	0.2 - 3.2	355-478	(2) in (1)
Skripka *et al.* (ref 23,28,30)	2 - 79	473,493	(2) in (1)
Price (ref 29)	-[a]	298-425	(1) in (2)
De Loos *et al.* (ref 39)	15 - 140	610-675	mutual
Tsonopoulos and Wilson (ref 40)	-[a]	313-473	mutual
Rebert and Hayworth (ref 41)	4.6 - 22.2	493-645	(1) in (2)
Roof (ref 42)	5.295[b]	495.2[b]	-[b]

[a] Along 3-phase equilibrium line.

[b] Critical point.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. October 1986.

CRITICAL EVALUATION: (continued)

As can be seen from Table 4, virtually none of the solubility data at elevated pressures have been obtained under comparable conditions, thus precluding evaluation of their reliability. However, it should be noted that the atmospheric pressure data of Kudchadker and McKetta (ref 13) disagree markedly from other studies. Also, the interpolated values of Burd and Braun (ref 18) and Skripka *et al.* (ref 28) at ~ 473K and ~ 3.2 MPa are in poor agreement (~ 3.2 and ~ 1.8 g(2)/100g sln respectively).

Roof and Scheffer have measured the temperature and pressure at the critical end point. Their values are in reasonable agreement (Table 4).

De Loos *et al.* (ref 39) have studied the two phase-one phase boundaries near but to the left of the critical line starting at the critical point of water (refer to Figure 3). Although the absence of confirmatory studies precludes Critical Evaluation the results are consistent with the phase behaviour of other alkane + water systems.

The interested user is referred to the original measurements in the data sheets for further information, bearing in mind that all values should be regarded as very tentative.

REFERENCES

1. Herz, W. *Chem. Ber.* 1898, *51*, 2669-72.
2. Scheffer, F.E.C. *Proc. Roy. Acad. Amsterdam* 1913, *16*, 404-18.
3. Führer, H. *Chem. Ber.* 1924, *57*, 510-5.
4. Milligan, L.H. *J. Phys. Chem.* 1924, *28*, 494-7.
5. Bennett, G.M.; Philip, W.G. *J. Chem. Soc.* 1928, 1937-42.
6. Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* 1948, *40*, 1491-3.
7. Gester, Jr., G.C. *Chem. Eng. Progr.* 1947, *43*, 117-22.
8. Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* 1948, *16*, 537-43.
9. Durand, R. *C.R. Hebd. Seances Acad. Sci.* 1948, *226*, 409-10.
10. McBain, J.W.; Lissant, K.F. *J. Phys. Chem.* 1951, *55*, 655-62.
11. McCants, J.F.; Jones, J.H.; Hopson, W.H. *Ind. Eng. Chem.* 1953, *45*, 454.
12. Jones, J.H.; McCants, J.F. *Ind. Eng. Chem.* 1954, *46*, 1956-8.
13. Kudchadker, A.P.; McKetta, J.J. *Petrol. Refiner* 1961, *40*, 231-2.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth., W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

REFERENCES (continued)

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

15. Zel'venskii, Ya.D.; Efremov, A.A.; Larin, G.M. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 3-7.

16. Barone, G.; Crescenzi, V.; Pispisa, B.; Quadrifoglio, F. *J. Macromol. Chem.* 1966, *1*, 761-71.

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

18. Burd, Jr., S.D.; Braun, W.G. *Proc. Div. Refining, Am. Petrol. Inst.* 1968, *48*, 464-76.

19. Nelson, H.D.; De Ligny, C.J. *Rec. Trav. Chim. Pays-Bas* 1968, *87*, 528-44.

20. Roddy, J.W.; Coleman, C.F. *Talanta* 1968, *15*, 1281-6.

21. Benkovski, V.G.; Nauruzov, M.H.; Bogoslovaskaya, T.M. *Tr. Inst. Khim. Nefti Prir. Solei Akad. Nauk Kaz. SSR* 1970, *2*, 25-32.

22. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-7.

23. Sultanov, R.G.; Skripka, V.E.; Deposited doc. VINITI 5347-72; *Zh. Fiz. Khim.* 1973, *47*, 1035.

24. Leinonen, P.J.; Mackay, D. *Can. J. Chem. Eng.* 1973, *51*, 230-3.

25. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.

26. Mackay, D.; Shiu, W.Y.; Wolkoff, A.W. Water Quality Parameters, ASTM STP 573, 1975, 251-8.

27. Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. Deposited doc. VINITI 438-76; *Zh. Fiz. Khim.* 1976, *50*, 1343.

28. Namiot, A.Yu.; Skripka, V.G.; Lotber, Yu.G. Deposited doc. VINITI 1213-76; *Zh. Fiz. Khim.* 1976, *50*, 2718.

29. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.

30. Skripka, V.G. *Tr. Vses Neftegazov. Nauch Issled. Inst.* 1976, *61*, 139-51.

31. Korenman, I.M.; Aref'eva, R.P. Patent USSR, 553 524, 1977, 04.05. *C.A. 87* : 87654.

32. Sugi, H.; Katayama, T. *J. Chem. Eng. Japan* 1977, *10*, 400-2.

33. Charykov, A.K.; Tikhomirov, V.I.; Potapova, T.M. *Zh. Obshch. Khim.* 1978, *48*, 1916-21.

34. Korenman, I.M.; Aref'eva, R.P. *Zh. Prikl. Khim.* 1978, *51*, 957-8.

35. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

36. Aquan-Yuen, M.; Mackay, D.; Shui, W.Y. *J. Chem. Eng. Data* 1979, *24*, 30-4.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

REFERENCES (continued)

37. Gill, S.J.; Nichols, N.F.; Wadso, I. *J. Chem. Thermodyn.* 1976, *8*, 445-52.

38. Jonsson, J.A.; Vejrosta, J.; Novak, J. *Fluid Phase Equil.* 1982, *9*, 279-86.

39. De Loos, Th.W.; Penders, W.G.; Lichtenthaler, R.N. *J. Chem. Thermodyn.* 1982, *14*, 83-91.

40. Tsonopoulos, C.; Wilson, G.M. *A. I. Ch. E. J.* 1983, *29*, 990-8.

41. Rebert, C.J.; Hayworth, K.E. *A. I. Ch. E. J.* 1967, *13*, 118-21.

42. Roof, J.G. *J. Chem. Eng. Data* 1970, *15*, 301-3.

43. Scott, R.L.; van Konynburg, P.H. *Phil. Trans. Roy. Soc.* London 1980, *A298*, 495.

44. Hicks, C.P.; Young, C.L. *Chem. Rev.* 1975, *75*, 119.

ACKNOWLEDGEMENTS

The Evaluator thanks Dr Brian Clare for the regression analyses and graphics and Dr Marie-Claire Haulait-Pirson for comments and a preliminary draft of the reference list. Section 3 was written jointly with C. L. Young, Department of Physical Chemistry, University of Melbourne, Australia.

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Fühner, H.

Ber. Dtsch. Chem. Ges. 1924, *57*, 510-5.

VARIABLES:

One temperature: 15.5°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 15.5°C was reported to be 0.022 mL(1)/100 mL sln or 0.014 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compiler is 2.92×10^{-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:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Black, C.; Joris, G.G.; Taylor, H.S.

J. Chem. Phys. 1948, *16*, 537-43.

VARIABLES:

One temperature: 20°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in hexane at 20°C and at a total saturation pressure of 1 atm was reported to be 0.0111 g(2)/100 g(1). The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 0.0111 g(2)/100 g sln and 5.3×10^{-4}.

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) Hexane; C_6H_{14}; 110-54-3 (2) Water; H_2O; 7732-18-5]	Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* 1948, *40*, 1491-3.
VARIABLES:	**PREPARED BY:**
One temperature: 25.0°C (298.2 K)	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of *n*-hexane in water at 25.0°C was reported to be <0.04 mL (1)/100 mL (2).

A similar result was reported for (1) in 40.0% (w/w?) aqueous sodium xylenesulfonate.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A known volume of water, typically 50 mL, was placed in a stoppered Babcock tube having a neck graduated from 0 to 1.6 mL in steps of 0.02 mL. An excess of solute was added and the mixture allowed to come to equilibrium in a constant temperature bath then centrifuged. The amount of solute dissolved was determined by subtracting the undissolved solute, measured directly in the tube, from the total added.

SOURCE AND PURITY OF MATERIALS:

1. "Highest grade commercial sample available"; no other details given.
2. Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Durand, R.

C.R. Hebd. Seances Acad. Sci. 1948, *226*, 409-10.

VARIABLES:

One temperature: 16°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 16°C was reported to be 0.055 $cm^3(1)/dm^3(2)$.
With the assumption of a solution density of 1.00 g cm^{-3} and a density value of 0.6629 g cm^{-3} for hexane at 16°C (ref 2), the corresponding mass percent is 0.0036 g(1)/100 g sln and the corresponding mole fraction, x_1, is 7.5 x 10^{-6} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The thermostatic method described in ref 1 was used.
Addition of pipetted volumes of (1) to (2) followed by shaking is repeated till appearance of turbidity.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) distilled.

ESTIMATED ERROR:

soly. ± 0.005 $cm^3(1)/dm^3(2)$.

REFERENCES:

1. Durand, R. *C.R. Hebd. Seances Acad. Sci.* 1946, *223*, 898-900.

2. Timmermans, J.; *Physico-chemical constants of pure organic compounds*, Elsevier, 1950.

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

McBain, J.W.; Lissant, K.J.

J. Phys. Colloid. Chem. 1951, *55*, 655-62.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be 0.012 g(1)/100 mL sln.

With the assumption of a solution density of 1.00 g cm^{-3}, the corresponding mass percent is 0.012 g(1)/100 g sln and the corresponding mole fraction, x_1, is 2.5×10^{-5} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

10 mL of (2) was pipetted into glass vials, following which, varying amounts of (1) were added to each bottle by direct weighing. The vials were shaken overnight. When two vials had been obtained, one clear and one with excess hydrocarbon and containing amounts differing by less than 1 mg, the two values were averaged and the mean taken as the amount solubilized.

SOURCE AND PURITY OF MATERIALS:

(1) C.P. grade.

(2) distilled and boiled to remove CO_2.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

McCants, J.F.; Jones, J.H.; Hopson, W.H.

Ind. Eng. Chem. 1953, *45*, 454-6.

VARIABLES:

One temperature: 100°F (311 K)

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of *n*-hexane in water at 100°F (311 K) was reported to be <0.1 g(1)/100 g sln. The corresponding mole fraction, x_2, calculated by the compiler, is $< 2 \times 10^{-4}$.

The solubility of water in *n*-hexane at 100°F (311 K) was reported to be <0.1 g(2)/100 g sln. The corresponding mole fraction, x_2, calculated by the compiler, is $< 5 \times 10^{-3}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was essentially that of ref. 1 and involved titration of the second component to the cloud point, in a constant temperature bath.

SOURCE AND PURITY OF MATERIALS:

1. Phillips; pure grade; used without further purification; n_D^{20} 1.3752.
2. Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Washburn, E.R.; Hnizda, V.; Vold, R.D. *J. Am. Chem. Soc.* 1931, *53*, 3232.

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Jones, J.H.; McCants, J.F.

Ind. Eng. Chem. 1954, *46*, 1956-8.

VARIABLES:

One temperature: 100°F

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 100°F (37.78°C) was reported to be 0.4 g(1)/100 g sln. The corresponding mole fraction, x_1, calculated by the compiler is 8.3×10^{-4}.
The solubility of water in hexane at 100°F (37.78°C) was reported to be 0.2 g(1)/100 g sln. The corresponding mole fraction, x_2, calculated by the compiler is 9.5×10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (2) in (1) was obtained by titrating (1), brought to 100°F. As the cloud point was approached, (2) was added dropwise and the flask agitated in the 100°F constant temperature bath. The solubility of (1) in (2) was determined by titrating (2) at 100°F with (1).

SOURCE AND PURITY OF MATERIALS:

(1) Phillips; used as received;
$n_D^{20} = 1.3745$
$d_4^{20} = 0.6607$

(2) distilled; $n_D^{20} = 1.3330$

ESTIMATED ERROR:

temp. ± 0.2°F

REFERENCES:

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Kudchadker, A.P.; McKetta, J.J.

Petrol. Refiner. 1961, *40*, 231-2.

VARIABLES:

Temperature: 100-280°F
Pressure: 24-525 psia

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of hexane in water

t/°F	T/ K (compiler)	p/psia	p/MPa (compiler)	10^4x_1	g(1)/100 g sln (compiler)
100	310.94	24.8	0.171	0.2214	0.01060
		41.2	0.284	0.302	0.01446
		74.9	0.516	0.319	0.01527
		101.1	0.697	0.342	0.01637
		133.8	0.923	0.339	0.01623
		220.2	1.518	0.342	0.01637
		308.5	2.127	0.3398	0.01627
		422.5	2.913	0.3396	0.01626
		513.0	3.537	0.342	0.01637
160	344.27	45.2	0.312	0.398	0.01905
		75.3	0.519	0.541	0.02590
		112.6	0.776	0.644	0.03083
		172.2	1.187	0.6349	0.03039
		252.0	1.737	0.633	0.03030
		338.6	2.335	0.64	0.03063
		432.2	2.980	0.648	0.03102
		488.1	3.365	0.64	0.03063

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus for producing equilibrium conditions and analytical procedure are the same as described in ref 1. No more details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; certified purity of at least 99.0 mole percent; used as received.

(2) distilled; boiled to remove any dissolved gases.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Davis, J.E. M.S. Thesis, The University of Texas, Austin, 1959.

(1) Hexane; C_6H_{14}; [110-54-3]

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

Kudchadker, A.P.; McKetta, J.J.

Petrol. Refiner. 1961, *40*, 231-2.

Solubility of hexane in water

t/°F	T/ K (compiler)	p/psia	p/MPa (compiler)	10^4x_1	g(1)/100 g sln (compiler)
220	377.60	80.3	0.554	0.394	0.01886
		116.6	0.804	0.608	0.02910
		174.8	1.205	0.87	0.04164
		233.3	1.609	1.08	0.05169
		282.5	1.948	1.092	0.05226
		355.1	2.448	1.112	0.05322
		444.4	3.064	1.09	0.05217
		524.8	3.618	1.11	0.05312
280	410.94	98.2	0.677	0.272	0.01302
		137.5	0.948	0.475	0.02274
		205.0	1.413	0.826	0.03953
		268.8	1.853	1.155	0.05527
		353.9	2.440	1.478	0.07072
		392.2	2.704	1.588	0.07598
		435.0	2.999	1.685	0.08062
		506.5	3.492	1.772	0.08478

COMPONENTS:

(1) Hexane, C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 20-40°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in hexane

t/°C	g(2)/100 g sln	10^4x_2 (compiler)
20	0.0101	4.83
30	0.0179	8.56
40	0.0317	15.15

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours 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:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Zel'venskii, Ya.D; Efremov, A.A.; Larin, G.M.

Khim. Tekhnol. Topl. Masel 1965, *10*, 3-7.

VARIABLES:

One temperature: 20°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in hexane at 20°C was reported to be 0.0166 g(2)/100 g sln.

The corresponding mole fraction, x_2, calculated by the compiler is 7.9×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturated solutions of tritium labeled (2) in (1) were prepared in two ways. In the first, nitrogen was passed through the vessel with (2) and next through the vessel with (1) and frozen. In the second, about 500 mL of (1) and 1 mL (2) were stirred. The concentration of (2) in (1) was calculated from scintillation measurements.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; pure grade; shaken with conc. H_2SO_4; washed with water, dried over sodium, and distilled; purity not specified. b.p. 68.81°C, m.p. -95.5°C.

(2) source not specified; commercial; 1 Ci/mL HTO used as received.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Barone, G.; Crescenzi, V.; Pispisa, B.; Quadrifoglio, F.

J. Macromol. Chem. <u>1966</u>, *1*, 761-71.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors report a value of 9.6×10^{-4} mol(1)/dm^3(2) for the solubility of hexane 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* = 149 mm Hg. The solubility at system pressure calculated by the compiler is 1.882×10^{-4} mol(1)/dm^3(2) and the corresponding mass percent and mole fraction, x_1, are 0.001621 g(1)/100 g sln and 3.385×10^{-6}.

The compiler's calculation assumes a solution density of 0.6629 g/mL (the density of hexane reported in ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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.

SOURCE AND PURITY OF MATERIALS:

(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:

1. Timmermans, J. *Physico-chemical constants of pure organic compounds*, Elsevier, 1950.

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be 9.5 mg (1)/kg sln (0.00095 g(1)/100 g sln).
The corresponding mole fraction, x_1, calculated by the compiler, is 1.99×10^{-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. 1.3 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:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Burd, S.D.; Braun, W.G.

Proc. Div. Refining, Am. Petrol. Inst. 1968, *48*, 464-76.

VARIABLES:

Temperature and pressure

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Hydrocarbon-rich liquid phase composition for the three-phase conditions.

p/psia	p/MPa (compiler)	t/°F	T/K (compiler)	g(2)/100 g sln	x_2 (compiler)
30	0.207	179	354.82	0.14	0.0067
60	0.414	223	379.26	0.32	0.0151
100	0.689	261	400.37	0.58	0.0272
150	1.034	292	417.59	0.91	0.0421
200	1.379	317	431.48	1.26	0.0575
250	1.724	337	442.59	1.62	0.0730
300	2.068	355	452.59	2.03	0.0902
350	2.413	369	460.37	2.35	0.1032
400	2.758	383	468.15	2.78	0.1294
42	0.290	200	366.48	0.21	0.0100
87	0.600	250	394.26	0.49	0.0230
165	1.138	300	422.04	1.03	0.0474
286	1.972	350	449.82	1.89	0.0844
470	3.241	400	477.59	3.30	0.1403

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The vapor and liquid phase compositions have been determined for the (1)-(2) system in the two-phase hydrocarbon-rich liquid region. Equilibrium points were obtained by incremental addition of water followed by stirring, settling, sampling and chromatographic analysis. This procedure was continued until addition of water resulted in no pressure increase, indicating three-phase conditions. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; 99.5% purity.

(2) laboratory distilled.

ESTIMATED ERROR:

soly. ± 0.004 weight fraction of the (2) present.

REFERENCES:

COMPONENTS:

1. Hexane; C_6H_{14}; [110-54-3]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rebert, C. J.; Hayworth, K. E.; *Am. Inst. Chem. Engnrs. J.* 1967, *13*, 118-121.

VARIABLES:

Pressure and temperature along one phase-two phase boundary.

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

Smoothed data

T/K	T/°C	P/MPa	p/psi	g (1)/100 g (soln.)	$x_{C_6H_{14}}$
603	330	12.90	1870	2.0	0.0042
613	340	14.67	2127		
623	350	16.65	2414		
633	360	18.83	2731		
643	370	21.46	3112		
644	371	21.77	3157		
645.0[a]	371.8	22.23	3223		
644	371	22.17	3214		
643	370	22.02	3193		
633	360	20.27	2939		
623	350	18.72	2715		
613	340	17.43	2527		
608	335	16.96	2459		
605	332	16.78	2433		
603	330	16.70	2422		
601	328	16.67	2417		
599	326	16.69	2420		
597	324	16.76	2430		
595	322	16.90	2450		
591	318	17.71	2568		
588	315	19.24	2790		
573	300	8.92	1294	15.4	0.0367
583	310	10.48	1520		
593	320	12.19	1768		

(cont.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Samples of mixtures of known composition confined over mercury. Samples heated in a vapor bath and the pressure-temperature phase boundaries determined by direct observation of appearance or disappearance of a phase. Apparatus similar to that described in ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. No details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.05$;

$\delta p/\mathrm{psi} = \pm 1$.

REFERENCES:

1. Rebert, C. J.; Kay, W. B. *Am. Inst. Chem. Engnrs. J.* 1959, *5*, 285.

COMPONENTS:

1. Hexane; C_6H_{14}; [110-54-3]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rebert, C. J.; Hayworth, K. E.
Am. Inst. Chem. Engnrs. J.
1967, *13*, 118-121.

EXPERIMENTAL VALUES:

Smoothed data

T/K	T/°C	P/MPa	p/psi	g (1)/100 g (soln.)	$x_{C_6H_{14}}$
598	325	13.13	1904	15.4	0.0367
603	330	14.11	2046		
608	335	14.88	2158		
613	340	16.13	2339		
618	345	17.23	2498		
623	350	18.41	2670		
628	355	19.74	2862		
633	360	21.31	3090		
543	270	7.08	1026	50.57	0.1762
548	275	7.62	1105		
553	280	8.25	1196		
558	285	8.94	1297		
563	290	9.71	1408		
568	295	10.55	1530		
573	300	11.45	1660		
578	305	12.40	1798		
583	310	13.42	1946		
588	315	14.62	2120		
593	320	16.03	2324		
598	325	17.63	2556		
603	330	19.53	2832		
608	335	21.63	3136		
493	220	4.63	672	85.34	0.5489
498	225	5.06	734		
503	230	5.52	800		
508	235	6.01	871		
513	240	6.53	947		
518	245	6.97	1011		
523	250	7.74	1123		
528	255	8.49	1231		
533	260	9.31	1350		
538	265	10.23	1484		
543	270	11.34	1645		
548	275	12.92	1873		
553	280	14.88	2158		
558	285	17.39	2522		

[a] Critical point.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-8] (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: 4-55°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of hexane in water

t/°C	10^6x_1	mg(1)/kg sln (compiler)
4.0	3.42 ± 0.34	16.4
14.0	3.17 ± 0.52	15.2
25.0	3.83 ± 0.47	18.3
35.0	2.69 ± 0.26	12.9
45.0	4.64 ± 0.72	22.2
55.0	4.42 ± 0.26	21.2

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) Fluka purum.

(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:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Roddy, J.W.; Coleman, C.F.

Talanta 1968, *15*, 1281-6.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in hexane at 25°C was reported to be 0.00362 mol(2) dm^{-3} sln corresponding to a mole fraction, x_2, of 4.76×10^{-4}. The corresponding mass percent value calculated by the compiler is 0.00995 g(2)/100 g sln.

The compiler's calculation assumes a solution density of 0.6629 g/mL (the density of hexane reported in ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A method of gravimetric absorption monitored by tritium tracer was used. (1) was equilibrated with a slight excess of tritiated water by shaking over a period of at least 8 hr in a thermostat. The phases were allowed to separate for at least 16 hr and then were sampled for tritium analysis. Most of the (1) phase was weighed into a boiling flask of a closed distillation system and then distilled through a magnesium perchlorate weighing tube. The magnesium perchlorate was then dissolved for measurement of its tritium content by liquid scintillation counting with a Packard Tri-Carb Scintillation Spectrometer.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99%; purified by shaking with concentrated sulphuric acid, washed with water and dried with sodium sulphate.

(2) tritiated water at 5 Ci/mL; New England Nuclear Corp.; diluted to about 1 mCi/mL.

ESTIMATED ERROR:

soly. better than 1% (type of error not specified)

REFERENCES:

1. Timmermans, J. *Physico-chemical constants of pure organic compounds*, Elsevier, 1950.

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Benkovski, V.G.; Nauruzov, M.H.; Bogoslovaskaya, T.M.

Tr. Inst. Khim. Nefti Prir. Solei Akad. Nauk Kaz. SSR 1970, *2*, 25-32.

VARIABLES:

One temperature: 303 K

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in hexane at 303 K was reported to be 0.0051 g(2)/100 g sln.

The corresponding mole fraction, x_2, value calculated by compiler is 0.00024.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equal volumes of (1) and (2) were placed in a glass cylinder and periodically shaken for 6 h, then sampled and analyzed by the Karl Fischer method.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; purified; purity not specified.

(2) distilled.

ESTIMATED ERROR:

Not specified

REFERENCES:

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Krasnoshchekova, P.Ya.;
Gubergrits, M.Ya.

Neftekhimiya 1973, *13*, 885-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be $x_1 = 2.8 \times 10^{-6}$.
The corresponding mass percent calculated by the compiler is 1.3×10^{-3} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigorously stirred magnetically for 10-12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP reagent; purity not specified.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS: (1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Leinonen, P.J.; Mackay, D. *Can. J. Chem. Eng.* 1973, *51*, 230-3.
VARIABLES: One temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be 12.3 mg(1)dm^{-3} sln corresponding to a mole fraction, x_1, of 2.5×10^{-6}.

The corresponding mass percent calculated by the compiler is 0.00123 g(1)/100 g sln.

The compiler's calculation assumes a solution density of 1.00 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was equilibrated for at least 12 hrs in a 200 mL Teflon stoppered vessel with gentle shaking. The solution was allowed to settle for 6 hrs and the aqueous phase was tested (Tyndall effect). Both phases were analysed by the gas chromatographic technique of internal standardization. The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analysed by GLC. The instrument was a Hewlett-Packard model equipped with a flame ionization detector.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; research grade; purity 99%+; used without further purification.

(2) doubly distilled.

ESTIMATED ERROR:

temp. ± 0.1 K
soly. ± 1 mg(1)dm^{-3} sln

REFERENCES:

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C-Y.

Can. J. Chem. 1973, *51*, 4018-23.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of hexane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0^a	16.5^c	3.44×10^{-6}
25^b	12.4^c	2.59×10^{-6}

Solubility of water in hexane

t/°C	mg(2)/kg sln	x_2 (compiler)
0^a	28^d	1.34×10^{-4}
25^b	90^e	4.30×10^{-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:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.J.; Wolkoff, A.W.

"Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. 1975, *573*, 251-8.

VARIABLES:

not specified

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported the value of 16.2 mg(1)dm^{-3} sln for the solubility of hexane in water. With the assumption of a solution density of 1.00 g cm^{-3}, the corresponding mass percent, calculated by the compiler, is 0.00162 g(1)/100 g sln and the corresponding mole fraction, x_1, is 3.4×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(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.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. ± 10% (compiler)

REFERENCES:

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S.

Zh. Fiz. Khim. 1976, *50*, 1344.
Deposited doc. 1976,
VINITI 438-76.

VARIABLES:

One temperature: 20°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of hexane in water at 20°C was reported to be $x_1 = 3 \times 10^{-6}$.

The corresponding mass percent calculated by the compiler is 0.0014 g(1)/100 g sln.

The solubility of water in hexane at 20°C was reported to be $x_2 = 3.7 \times 10^{-4}$.

The corresponding mass percent calculated by the compiler is 0.0077 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by Karl Fischer reagent method.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; pure or analytical reagent grade; purity <99.9%.

(2) not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Namiot, A.Yu.; Skripka, V.G.; Lotter, Yu.G.

Zh. Fiz. Khim. 1976, *50*, 2718
Deposited doc. 1976,
VINITI 1213-76.

VARIABLES:

Temperature: 200 and 220°C
Pressure: 2.0-5.2 MPa

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in hexane

t/°C	p/kg cm^{-2}	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
200	20	2.0	0.006	0.13
200	25	2.5	0.024	0.51
200	30	2.9	0.051	1.11
200	35	3.4	0.084	1.92
200	37	3.6	0.097	2.2
220	25	2.5	0.002	0.04
220	30	2.9	0.023	0.49
220	35	3.4	0.053	1.16
220	40	3.9	0.088	1.98
220	45	4.4	0.129	3.00
220	50	4.9	0.179	4.36
220	53.3	5.2	0.216	5.44

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The static method for vapor-liquid equilibrium described in ref 1 was used.
No more details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP reagent; used as received.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Sultanov, R.G.; Skripka, V.G.; Namiot, Yu.A. *Zh. Fiz. Khim.* 1976, *46*, 2170.

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

Temperature: 25-151.8°C

PREPARED BY:

F. Kapuku

EXPERIMENTAL VALUES:

Solubility of hexane in water at system pressure

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
25.0	9.47 ± 0.20	0.000947	1.98
40.1	10.1 ± 0.3	0.00101	2.11
55.7	13.2 ± 0.5	0.00132	2.76
69.7	15.4 ± 1.9	0.00154	3.22
69.7	15.2 ± 0.5	0.00152	3.18
99.1	22.4 ± 1.0	0.00224	4.68
114.4	29.2 ± 1.0	0.00292	6.10
121.3	37.6 ± 1.2	0.00376	7.86
137.3	56.9 ± 2.3	0.00569	11.89
151.8	106.0 ± 4.0	0.0106	22.2

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 insured 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:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Skripka, V.G.
Tr. Vses. Neftegazov. Nauch. Issled. Inst. 1976, *61*, 139-51.

Sultanov, R.G.; Skripka, V.E.
Zh. Fiz. Khim. 1973, *47*, 1035.
Deposited doc. 1976, VINITI 5347-72

VARIABLES:

Temperature: 200 and 220°C
Pressure: 3.6-78.5 MPa

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in hexane

t/°C	p/kg cm^{-2}	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
200	37	3.6	0.097	2.20
	50	4.9	0.094	2.12
	100	9.8	0.084	1.88
	200	19.6	0.072	1.60
	300	29.4	0.065	1.43
	400	39.2	0.060	1.32
	500	49.0	0.055	1.20
	600	58.8	0.051	1.11
	700	68.6	0.047	1.02
	800	78.5	0.041	0.89
220	50.8	5.0	0.187	4.59
	80	8.3	0.145	3.42
	100	9.8	0.134	3.13
	200	19.6	0.113	2.59
	300	29.4	0.102	2.32
	400	39.2	0.092	2.07
	500	49.0	0.083	1.86
	600	58.8	0.074	1.64
	700	68.6	0.068	1.50
	800	78.5	0.065	1.43

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The experimental technique was described in ref 1. No details reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified, chemical reagent grade; purity not specified; used as received.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. *Gazov. Prom.* 1971, *4*, 6.

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

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 hexane in water at 20°C was reported to be 0.14 g(1)dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.014 g(1)/100 g sln and 2.9×10^{-5}.

The compiler's calculation assumes a solution density of 1.00 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS: (1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Sugi, H.; Katayama, T. *J. Chem. Eng. Jap.* <u>1977</u>, *10*, 400-2.
VARIABLES: One temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in hexane at 25°C was reported to be in mole fraction, $x_2 = 5.1 \times 10^{-4}$. The corresponding mass percent calculated by the compiler is 0.01066 g (2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The Karl Fischer method was used. The experimental apparatus and procedures are given in ref 1.	**SOURCE AND PURITY OF MATERIALS:** (1) Merck Uvasol spectrograde chemical; used without further purification. (2) deionized and fractionated twice in an all-glass distillation flask.
	ESTIMATED ERROR: not specified.
	REFERENCES: 1. Sugi, H.; Nitta, T.; Katayama, T. *J. Chem. Eng. Jap.* <u>1976</u>, *9*, 12.

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Charykov, A.K.; Tikhomirov, V.I.; Potapova, T.M.

Zh. Obshch. Khim. 1978, *48*, 1916-21.

VARIABLES:

One temperature: 20°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in hexane at 20°C was reported to be 0.0035 mol(2) dm^{-3} sln corresponding to a mole fraction, x_2, of 0.00046. The mass percent calculated by the compiler is 0.0084 g(2)/100 g sln. The compiler's calculation assumes a solution density of 0.663 g/mL (the density of hexane reported in ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturation of (1) with (2) was obtained by shaking definite volumes of (1) and (2) in a mechanical shaker for 2-3 hrs. (2) was determined in an aliquot (0.2-5 mL) of (1) by the Karl Fischer method. No more details are given.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Timmermans, J. *Physico-chemical constants of pure organic compounds*, Elsevier, 1950.

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Korenman, I.M.; Aref'eva, R.P.

Zh. Prikl. Khim. 1978, *51*, 957-8.

VARIABLES:

Temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be 0.16 g(1)dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.016 g(1)/100 g sln and 3.3×10^{-5}.

The compiler's calculation assume a solution density of 1.00 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

About 200-500 mL(2) was placed in a ground-joint glass cylinder and 20-50 mg of an insoluble indicator (dithizon, phenolphthalein, etc.) was added, and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall above the liquid layer. Blanks were made to determine the excess of (1).

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.01 g(1)dm^{-3} sln (standard deviation from 6 determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water, H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *12*, 413-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be 9.47 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 9.47×10^{-4} g(1)/100 g sln and 1.98×10^{-6}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.	(1) not specified. (2) not specified. **ESTIMATED ERROR:** soly. 0.3 mg(1)/kg(2) (standard deviation from 7-9 determinations) **REFERENCES:**

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Aquan-Yuen, M.; Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1979, *24*, 30-4.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be 0.0123 g(1) dm^{-3} sln.
With the assumption of a solution density of 1.00 g cm^{-3}, the corresponding mass percent is 0.00123 g(1)/100 g sln and the corresponding mole fraction, x_1, is 2.57 x 10^{-6} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturated solutions were prepared by adding an excess of (1) in (2) for 24 h, followed by settling in the water-bath for at least 48 hrs. The dissolved (1) was extracted by helium and trapped in liquid nitrogen. (1) was then injected into the GC column. The gas chromatograph was a Hewlett-Packard Model equipped with a flame ionization detector. The technique is described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) Fisher Scientific; pure grade (99 mol%).

(2) not specified.

ESTIMATED ERROR:

soly. ± 0.0004 g(1) dm^{-3} sln (type of error not specified).

REFERENCES:

1. Mackay, D.; Shiu, W.Y. *Bull. Environ. Contam. Toxicol.* 1974, *15*, 101.

COMPONENTS:

1. Hexane; C_6H_{14}; [110-54-3]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

De Loos, Th. W.; Penders, W. G.;
Lichtenthaler, R. N.
J. Chem. Thermodyn.
1982, *14*, 83-91.

VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.	T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.
631.5	18.33	0.005	2.4	623.1	19.63	0.005	2.4
633.8	18.82			620.7	19.37		
635.9	19.31			618.3	19.23		
637.7	19.80			616.4	19.15		
639.7	20.27			614.8	19.10		
641.4	20.76			613.4	19.10		
643.5	21.25			610.9	19.20		
644.8	21.74			609.5	19.20		
645.5	22.08			608.4	19.25		
645.4	22.20			607.5	19.40		
645.3	22.22			606.3	19.45		
644.2	22.23			605.1	19.66		
643.3	22.18			604.2	19.80		
642.1	22.08			603.2	20.00		
641.2	21.99			601.8	20.30		
640.0	21.89			600.4	20.63		
640.0	21.78			597.6	21.92		
639.7	21.35			596.7	22.41		
634.6	21.13			596.3	24.69		
632.4	20.73			595.9	25.25		
628.4	20.34			595.9	26.23		
625.1	19.97						

(cont.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static visual cell fitted with magnetic stirrer. Composition of homogeneous phase determined from weighing cell charge at ambient temperature. Details of cell and procedure given in ref.(1). Pressure measured with a pressure balance and temperature measured with Pt resistance thermometer.

SOURCE AND PURITY OF MATERIALS:

1. Merck sample, purity at least 99.0 moles per cent. Degassed.
2. Doubly distilled. Conductivity less than 10^{-6} S cm^{-1}.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$ K;
$\delta P/MPa = \pm 0.02$ up to 40 MPa,
±0.05 above 40 MPa;
$\delta x = \pm 0.002$.

REFERENCES:

1. De Loos, Th. W.; Wijen, A. J. M.; Diepen, G. A. M. *J. Chem. Thermodyn.* 1980, *12*, 193.

COMPONENTS:

1. Hexane; C_6H_{14}; [110-54-3]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

De Loos, Th. W.; Penders, W. G.;
Lichtenthaler, R. N.
J. Chem. Thermodyn.
1982, *14*, 83-91.

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.	T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.
629.9	18.33	0.015	6.8	635.8	23.22	0.025	10.9
632.0	18.82			635.0	23.35		
634.9	19.56			633.8	23.53		
637.7	20.29			633.2	23.62		
639.3	20.76			632.6	23.72		
641.1	21.25			631.6	23.92		
642.7	21.99			630.2	24.46		
643.0	22.23			628.1	25.00		
642.4	22.47			627.1	25.40		
641.8	22.52			626.4	25.79		
641.6	22.54			626.2	25.94		
641.3	22.57			626.1	26.18		
641.2	22.58			625.6	26.68		
640.8	22.60			625.1	27.17		
637.4	22.74			624.9	27.65		
635.4	22.79			624.8	28.15		
633.5	22.86			624.6	29.12		
629.5	22.94			624.4	30.10		
627.9	23.01			624.5	31.09		
626.3	23.05			624.5	32.56		
624.8	23.15			624.9	33.54		
620.8	24.48			625.2	35.50		
620.3	24.72			625.9	36.97		
619.5	24.97			627.2	40.21		
618.3	25.21			629.0	45.08		
617.2	26.10			633.2	54.89		
616.9	29.64			638.8	64.68		
616.5	31.89			643.9	74.46		
616.6	34.54			649.4	86.68		
617.9	40.23			657.6	101.40		
622.9	59.82			663.1	118.56		
633.5	74.49			669.5	135.70		
639.0	86.73			635.8	21.02	0.030	12.9
645.1	106.32			636.2	21.18		
650.7	118.56			636.9	21.56		
655.4	129.84			637.4	21.71		
629.6	18.84	0.025	10.9	637.9	22.01		
630.7	19.06			638.0	22.35		
631.6	19.31			638.0	22.74		
632.5	19.56			637.5	22.84		
634.3	20.04			637.0	22.99		
635.1	20.29			636.6	23.08		
636.7	20.78			636.3	23.13		
638.0	21.19			636.0	23.20		
639.5	21.74			635.7	23.23		
640.1	22.23			635.6	23.28		
639.4	22.58			635.2	23.33		
639.3	22.63			634.9	23.43		
638.9	22.72			634.3	23.53		
638.4	22.82			633.3	23.72		
637.8	22.94			632.9	23.82		
637.5	22.99			632.5	23.92		
637.1	23.03			632.2	24.01		
636.8	23.08			631.9	24.12		
636.5	23.13			631.5	24.22		
636.1	23.18						

(cont.)

COMPONENTS:

1. Hexane; C_6H_{14}; [110-54-3]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

De Loos, Th. W.; Penders, W. G.;
Lichtenthaler, R. N.
J. Chem. Thermodyn.
1982, *14*, 83-91.

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.	T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.
631.0	24.31	0.030	12.9	632.1	20.78	0.042	17.3
630.8	24.41			633.3	21.27		
630.5	24.51			634.2	21.76		
630.0	24.60			635.0	22.25		
629.8	24.70			635.3	22.74		
629.5	24.80			634.7	23.13		
628.1	25.43			633.9	23.48		
627.1	26.08			632.4	24.01		
626.5	26.68			631.9	24.22		
626.3	27.17			631.5	24.31		
626.1	27.65			631.3	24.41		
626.0	27.85			631.2	24.46		
625.8	28.24			631.1	24.51		
625.7	28.83			631.0	24.55		
625.4	30.10			630.8	24.62		
625.5	30.89			630.0	24.95		
625.6	31.38			628.6	25.82		
625.7	31.78			627.8	26.50		
625.9	32.17			627.5	26.92		
626.3	33.05			627.3	27.27		
627.4	35.99			627.1	27.65		
627.9	37.22			626.8	28.15		
629.0	40.18			626.7	28.63		
637.0	57.34			626.6	29.12		
620.0	17.14	0.038	15.9	626.6	30.10		
624.1	18.11			626.7	31.09		
626.9	18.84			626.9	32.07		
630.0	19.82			627.2	33.54		
631.7	20.29			628.8	36.94		
633.8	21.02			629.2	38.31		
635.3	21.76			631.4	42.63		
636.0	22.25			633.7	47.53		
635.8	22.74			639.1	57.23		
635.8	22.89			643.9	66.12		
635.6	22.99			648.7	74.44		
634.7	23.23			655.9	88.41		
632.9	23.72			659.8	96.49		
632.3	23.82			664.4	106.30		
632.0	23.96			671.2	122.95		
631.7	24.06			616.3	16.65	0.049	19.8
630.9	24.26			618.3	17.02		
630.1	24.72			622.3	18.06		
629.1	25.21			623.4	18.35		
627.9	26.18			626.6	19.23		
627.1	27.17			628.4	19.80		
626.5	28.15			629.9	20.29		
626.2	29.62			631.4	20.78		
626.3	31.57			632.0	21.02		
627.0	33.54			632.5	21.27		
628.0	37.46			633.0	21.51		
632.2	45.08			633.4	21.76		
641.1	622.22			633.8	22.01		
625.0	18.59	0.042	17.3	633.9	22.10		
626.7	19.08			634.1	22.99		
628.3	19.56			634.0	23.08		
630.8	20.29			634.0	23.18		

(cont.)

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hexane; C_6H_{14}; [110-54-3] 2. Water; H_2O; [7732-18-5]	De Loos, Th. W.; Penders, W. G.; Lichtenthaler, R. N. *J. Chem. Thermodyn.* 1982, *14*, 83-91.

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.	T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.
633.5	23.43	0.049	19.8	629.9	25.29	0.060	23.4
633.2	23.58			628.8	26.26		
632.6	23.82			628.3	26.90		
632.3	23.96			628.1	27.46		
632.0	24.12			627.9	27.85		
631.0	24.55			627.8	28.24		
630.5	24.79			627.7	28.83		
630.1	24.90			627.7	29.42		
629.8	25.05			627.6	30.20		
629.8	25.15			627.7	30.89		
629.4	25.38			627.8	31.57		
629.0	25.63			628.1	32.56		
628.9	25.77			628.3	33.52		
628.6	26.02			628.7	34.50		
628.2	26.41			629.7	36.94		
627.5	27.22			631.5	40.18		
627.3	28.32			635.0	47.05		
627.3	29.62			641.9	56.82		
627.4	30.60			647.7	68.33		
627.6	31.57			653.5	78.63		
627.8	32.07			660.1	91.45		
628.0	32.80			663.9	98.94		
628.6	34.50			618.9	18.25	0.070	26.5
629.1	35.47			619.3	18.35		
629.4	36.50			620.1	18.59		
629.6	36.84			621.0	18.84		
630.1	37.93			622.5	19.33		
631.4	40.18			626.1	20.70		
633.0	42.38			627.3	21.34		
634.0	45.08			628.6	22.15		
641.2	57.56			629.3	22.74		
643.2	60.75			629.4	23.53		
648.3	69.54			629.2	24.12		
653.0	78.36			628.9	24.54		
653.8	79.35			628.6	25.00		
657.7	86.68			628.4	25.52		
665.9	102.87			627.9	26.18		
618.5	17.61	0.060	23.4	627.5	27.17		
620.3	18.11			627.3	28.15		
621.2	18.35			627.2	29.12		
622.9	18.84			627.3	30.10		
625.9	19.82			627.5	31.09		
627.7	20.56			627.8	31.07		
628.4	20.78			628.0	33.05		
629.5	21.27			628.3	34.00		
630.0	21.51			628.7	34.99		
630.6	21.76			628.6	34.50		
631.2	22.25			631.6	40.18		
631.6	22.74			634.4	45.08		
631.8	22.94			643.7	59.79		
631.9	23.53			652.9	74.44		
631.7	23.92			660.7	86.68		
631.4	24.12			616.3	17.78	0.081	29.7
631.2	24.31			617.3	18.13		
630.9	24.55			619.0	18.40		
630.5	24.95			621.3	19.33		

(cont.)

COMPONENTS:

1. Hexane; C_6H_{14}; [110-54-3]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

De Loos, Th. W.; Penders, W. G.;
Lichtenthaler, R. N.
J. Chem. Thermodyn.
1982, *14*, 83-91.

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.	T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.
622.8	19.82	0.081	29.7	628.5	34.50	0.094	33.2
624.0	20.31			630.5	37.93		
625.2	20.80			633.3	42.63		
626.1	21.29			634.8	45.08		
627.0	21.78			637.8	49.98		
627.6	22.27			641.0	54.87		
628.3	23.23			644.4	59.72		
628.3	24.22			645.9	62.22		
628.2	25.19			647.1	64.68		
628.0	25.70			653.3	74.44		
627.5	26.68			660.1	86.68		
627.4	27.65			667.9	101.40		
627.3	28.63			673.9	111.20		
627.4	29.62			613.4	17.98	0.102	35.2
627.7	30.60			613.8	18.03		
627.9	31.57			614.5	18.37		
628.2	32.54			615.2	18.61		
628.5	33.52			616.1	18.86		
629.0	34.50			617.4	19.35		
629.7	35.47			618.7	19.82		
630.1	36.94			619.8	20.31		
631.0	38.41			621.1	20.80		
632.1	40.18			622.0	21.29		
632.3	40.67			623.4	22.27		
632.8	41.40			624.1	22.96		
633.1	41.90			624.9	23.74		
633.5	42.63			625.3	24.72		
633.8	43.12			625.6	25.94		
634.3	43.85			625.9	27.17		
645.0	60.26			626.4	28.63		
647.2	64.66			626.7	30.10		
650.1	69.54			627.1	31.09		
654.5	76.79			627.5	32.07		
657.9	83.02			627.9	33.05		
662.7	92.08			628.9	34.50		
665.4	98.94			630.0	36.94		
671.2	108.75			632.8	41.40		
671.7	109.98			643.9	59.77		
608.9	16.65	0.094	33.2	652.9	74.44		
612.1	17.47			653.1	74.44		
615.0	18.37			653.5	75.67		
618.3	19.33			654.2	76.90		
619.5	19.77			660.0	86.68		
621.1	20.31			666.6	98.94		
621.5	20.55			610.2	18.08	0.119	39.3
622.1	20.80			613.1	19.10		
622.8	21.29			614.2	19.84		
623.8	21.78			617.7	21.12		
624.6	22.27			618.7	21.78		
625.6	23.25			620.5	23.01		
626.0	24.72			621.4	23.74		
626.1	25.70			622.1	24.48		
626.3	27.17			622.6	25.21		
626.6	29.62			623.2	26.18		
627.0	31.09			623.6	27.17		
627.6	32.56			624.2	28.15		
628.1	33.54						

(cont.)

COMPONENTS:

1. Hexane; C_6H_{14}; [110-54-3]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

De Loos, Th. W.; Penders, W. G.;
Lichtenthaler, R. N.
J. Chem. Thermodyn.
1982, *14*, 83-91.

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.	T/K	*P*/MPa	Mole fraction of hexane	g (1)/ 100 g soln.
624.6	29.12	0.119	39.3	616.8	21.31	0.135	42.7
625.1	30.10			617.7	21.60		
625.7	31.09			618.4	22.27		
626.2	32.07			619.1	22.76		
627.0	33.54			620.3	23.74		
627.6	34.52			621.0	24.72		
628.3	35.47			622.2	26.18		
629.4	37.43			622.9	27.17		
631.3	40.18			623.4	28.15		
632.9	42.63			624.1	29.12		
635.4	46.55			624.9	30.60		
637.7	49.98			625.8	32.07		
642.5	57.32			627.3	34.52		
645.6	62.22			628.2	35.96		
648.6	67.09			629.4	37.93		
652.7	74.44			631.2	40.18		
656.8	81.79			632.7	42.63		
662.3	91.59			634.2	45.08		
667.2	101.40			635.9	47.53		
672.1	111.20			643.7	59.77		
608.3	17.87	0.135	42.7	647.0	64.68		
609.1	18.13			653.1	74.44		
609.8	18.37			659.9	86.68		
611.3	18.86			666.5	98.94		
615.0	20.33			672.6	111.20		
616.0	20.82						

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

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

ORIGINAL MEASUREMENTS:

Jonsson, J.A.; Vejrosta, J.; Novak, J.

Fluid Phase Equil. 1982, *9*, 279-86.

VARIABLES:

Temperature: 15-35°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

	Solubility of hexane in water		
t/°C	mg(1)/kg sln	10^3g(1)/100g sln (compiler)	$10^6 x_1$ (compiler)
15	10.72	1.07	2.24
20	10.32	1.03	2.15
25	10.09	1.01	2.11
30	10.02	1.00	2.09
35	10.10	1.01	2.11

[a] Solubility values were calculated by the authors from their smoothed air-water partition coefficient (K_{AW}) by assuming K_{AW} values obtained at infinite dilution were valid at the saturation pressure of (1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Air-water partition coefficients were measured by saturating a portion of water by a stream of nitrogen containing a known vapour concentration of (1). After equilibration, the dissolved (1) was adsorbed in a porous polymer trap and the entrapped (1) analysed by gas chromatography. The method and apparatus are described in detail in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka, > 99.7%, used as received.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Vejrosta, J.; Novak, J.; Jonsson, J.A. *Fluid Phase Equil.* 1982, *8*, 25-35.

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]
(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Tsonopoulos, C.; Wilson, G.M.
A. I. Ch. E. J. 1983, *29*, 990-9.

VARIABLES:

Temperature: 311-473 K
Pressure: 0.05-3.5 MPa

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of hexane in water

T/K	p^{a}/MPa	$10^{4}\ x_1$	10^{2} g(1)/100 g sln (compiler)
310.93	–^{a}	0.238	0.114
366.48	–^{a}	0.573	0.274
367.55	–^{a}	0.535	0.256
373.15	0.3482	0.621	0.297
422.04	–^{a}	2.71	1.30
423.15	1.2548	3.39	1.62
473.15	3.516	18.5	8.85

a Not specified.

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

All experimental details are given in an Appendix deposited in a Documentation Centre rather than in the original paper. The solubility of (1) in (2) was measured by gas chromatography, whilst that of (2) in (1) was measured by Karl Fischer titration.

SOURCE AND PURITY OF MATERIALS:

(1) No details given

(2) No details given

ESTIMATED ERROR:

soly. ± 5% relative; repeatability of replicate analyses.
temp. not stated.
press. ± 1%; type of error not stated.

REFERENCES:

(1) Hexane; C_6H_{14}; [110-54-3]
(2) Water; H_2O; [7732-18-5]

(continued)

The solubility of water in hexane

T/K	p^a/MPa	$10^2\ x_2$	g(2)/100 g sln (compiler)
313.15	0.04537	0.117,0.123	0.025[b]
367.55	-[a]	0.595	0.124
373.15	0.3482	0.709	0.148
423.15	1.2548	3.11	0.667
473.15	3.516	11.0	2.52

[a] Not specified.
[b] Average value.

The three phase critical point was reported to be 496.7 K, 5.295 MPa and $x_1 = 4.982 \times 10^{-4}$ (0.238 g(1)/100 g sln, compiler).

The authors also report equations fitted to their own and literature data over the range 273-497 K, *viz.*

$$\ln x_1 = -367.9847 + 16128.646/T + 52.820813 \ln T$$

$$\ln x_2 = -45.1714 - 1635.73/T + 7.53503 \ln T$$

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

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

Authors	Method	Salinity g salts/kg sln	g(1)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC	6	7.55×10^{-3}
Aquan-Yuen *et al.* (ref 2)	Spectrofluorometry	35.3	7.86×10^{-4}

These two determinations were made at somewhat different salinities and thus cannot be directly compared. Because the presence of sea salts is expected to depress the solubility value below the value for pure water (tentative value 1.3×10^{-3} g(1)/100 g sln) the tentative value of 7.86×10^{-4} g(1)/100 g sln is adopted for hexane in seawater at the indicated temperature and salinity. The value of Krasnoshchekova and Gubergrits is considered doubtful. Freegarde *et al.* (ref 3) also measured the solubility of hexane in seawater. However, since they did not report temperature or salinity, their work is rejected. Aquan-Yuen *et al.* have also measured solubility over a range of salinities.

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

T/K	g salts/kg sln	g(1)/100 g sln
298	35.3	7.86×10^{-4}

REFERENCES

1. Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-8.
2. Aquan-Yuen, M.; Mackay, D; Shiu, W.Y. *J. Chem. Eng. Data* 1979, *24*, 30-4.
3. Freegarde, M.; Hatchard, C.G.; Parker, C.A. *Lab. Pract.* 1971, *20*, 35-40.

COMPONENTS:

(1) Hexane; C_6H_{14}; [110-54-3]

(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 hexane in seawater was reported to be 7.55×10^{-3} g(1)/100 g sln and the corresponding mole fraction, $x_1 = 1.3 \times 10^{-5}$.

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) Hexane; C_6H_{14}; [110-54-3]

(2) Sodium chloride; NaCl; [7647-14-5]

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

ORIGINAL MEASUREMENTS:

Aquan-Yuen, M.; Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1979, *24*, 30-4.

VARIABLES:

One temperature: 25°C

Salinity: 18-130 g(2)/kg sln.

PREPARED BY:

M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

Solubility of hexane in aqueous NaCl

mol(2)/L sln	g(2)/kg sln^a	mg(1)/L sln	10^4mass%(1)^a	$10^6 x_1$^{a}
0.31	17.9	10.48	10.35	2.19
0.62	35.3	8.06	7.86	1.68
1.00	56.2	7.54	7.25	1.58
1.50	82.6	4.88	4.60	1.08
2.00	108.2	3.75	3.47	0.846
2.50	132.7	2.55	2.32	0.583

'a' calculated by compilers

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturated solutions were prepared by adding excess (1) to a previously prepared salt solution. The resulting mixture was stirred for 24 hours and then allowed to settle for 48 hours. An aliquot was extracted with cyclohexane which was then analyzed spectrofluorometrically.

SOURCE AND PURITY OF MATERIALS:

(1) 99% pure from Fisher Scientific.

(2) reagent grade.

ESTIMATED ERROR:

soly ± 1 relative %.

REFERENCES: