COMPONENTS:	EVALUATOR:
(1) Propane; C_3H_8; [74-98-6] and (1) n-Butane; C_4H_{10}; [106-97-8] (2) Water-d_2; D_2O; [7789-20-0]	Rubin Battino Department of Chemistry Wright State University Dayton, Ohio 45435 U.S.A. November, 1983

CRITICAL EVALUATION:

The propane/D_2O and n-butane/D_2O systems were both studied by Kresheck et al. (1) and the n-butane/D_2O system was also studied by Ben-Naim et al. (2). The propane/D_2O data were smoothed to give:

$$\ln x_1 = -117.403 + 167.481/T + 46.4577 \ln T \quad \text{where } T = T/100 \text{ K} \quad (1)$$

The standard deviation in $\ln x_1$ was 0.0029 or about 0.3% in x_1. In smoothing the n-butane/D_2O data the two highest points from reference (2) were rejected. The resulting smoothing equation is:

$$\ln x_1 = -134.697 + 193.517/T + 54.1240 \ln T \quad \text{where } T = T/100 \text{ K.} \quad (2)$$

The standard deviation was 0.014 in $\ln x_1$ or about 1.4% in x_1. Smoothed data at 5 K intervals are given in the table below. The mole fractions are at 0.101325 MPa partial pressure of gas. The thermodynamic functions are for the transfer of the gas from the vapor phase at 0.101325 MPa partial pressure of gas to the (hypothetical) solution of unit mole fraction. The value of $\Delta \overline{C}_{p1}^{\circ}$ was constant at 386 J mol^{-1} K^{-1} for propane /D_2O and 450 J mol^{-1} K^{-1} for n-butane/D_2O. If required, values of $\Delta \overline{G}_1^{\circ} = -RT \ln x_1$ can be calculated from the smoothed mole fractions.

T/K	Propane $10^5 x_1$	n-Butane $10^5 x_1$	Propane $\Delta \overline{H}_1^{\circ}$/ kJ mol^{-1}	n-Butane $\Delta \overline{H}_1^{\circ}$/ kJ mol^{-1}	Propane $\Delta \overline{S}_1^{\circ}$/ J mol^{-1} K^{-1}	n-Butane $\Delta \overline{S}_1^{\circ}$/ J mol^{-1} K^{-1}
273.15	8.229	7.579	-33.74	-37.98	-201.7	-217.7
278.15	6.348	5.796	-31.81	-35.73	-194.7	-209.6
283.15	5.016	4.450	-29.88	-33.48	-187.8	-201.5
288.15	4.053	3.506	-27.95	-31.23	-181.1	-193.7
293.15	3.345	2.829	-26.02	-28.98	-174.4	-185.9
298.15	2.815	2.336	-24.08	-26.73	-167.9	-178.3
303.15	2.414	1.970	-22.15	-24.48	-161.5	-170.8
308.15	2.106	1.695	-20.22	-22.23	-155.2	-163.5
313.15	1.868	1.486	-18.29	-19.98	-148.9	-156.2
318.15	1.682	1.326	-16.36	-17.73	-142.8	-149.1
323.15	1.537	1.203	-14.43	-15.48	-136.8	-142.1
328.15	—	1.109	—	-13.23	—	-135.2

References

1. Kresheck, G.C.; Schneider, H.; Scheraga, H.A., *J. Phys. Chem.*, 1965, *69*, 3132-44.

2. Ben-Naim, A.; Wilf, J.; Yaacobi, M., *J. Phys. Chem.*, 1973, *77*, 95-102.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propane; C_3H_8; [74-98-6] (2) Water-d_2; D_2O; [7789-20-0]	Kresheck, G. C.; Schneider, H. Scheraga, H. A. *J. Phys. Chem.* 1965, *69*, 3132-44.
VARIABLES: T/K = 277.15 - 323.15 p_1/kPa = 101.325	PREPARED BY: H. L. Clever

EXPERIMENTAL VALUES:

Temperature		Mol Fraction[a]	Molarity	Molality
$t/^0C$	T/K	$10^5 x_1$	$10^3 c_1/\text{mol dm}^{-3}$	$10^3 m_1/\text{mol kg}^{-1}$
4	277.15	6.610, 6.744		
	277.15[b]	6.68 ± 0.07	3.68 ± 0.03	3.33 ± 0.03
10	283.15	5.021		
15	288.15	4.053, 4.064		
20	293.15	3.333		
25	298.15	2.819, 2.834		
	298.15[b]	2.83 ± 0.01	1.56 ± 0.01	1.41 ± 0.01
30	303.15	2.409		
35	308.15	2.096, 2.109		
40	313.15	1.871		
45	318.15	1.685, 1.691		
50	323.15	1.530, 1.537		
	323.15[b]	1.54 ± 0.01	0.84 ± 0.00	0.76 ± 0.00

[a] The experimental values of the mole fraction solubility were
    provided by H. Schneider. The last digit in each figure is not
    significant.

[b] Smoothed values from the original paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A known quantity of the gas was introduced from a gas buret into a calibrated volume which contained a weighed quantity of water. The water was stirred until equilibrium was attained (3 to 4 hours). The amount of gas in the vapor phase at equilibrium was determined from the partial pressure of the propane and volume of the vapor space. The volume was the difference in the empty vessel volume and the water volume. The amount of dissolved gas was obtained by difference.

The D_2O density values used were based on literature data (1). The gas volume was corrected for non-ideal behavior by use of a compressibility factor (2). At each temperature the solubility was usually measured at two partial pressures which ranged from 0.5 to 0.7 atm at 4 ^0C and 1.2 to 1.6 atm at 50 ^0C. All solubility data were normalized to a partial pressure of 1 atm.

SOURCE AND PURITY OF MATERIALS:

(1) Propane. Matheson Co., Inc.
    99.92 mole per cent.

(2) Water-d_2. US Atomic Energy
    Commission. 99.7 mol per cent
    D_2O.

ESTIMATED ERROR:

$\delta x_1/x_1$ = ± 0.005

REFERENCES:
1. Steckel, F.; Szapiro, S.
    Trans. Faraday Soc. 1963, *59*, 331.

2. Silberberg, I. H.; Kuo, P. K.;
    McKetta, J. J.
    Petrol. Engr. 1954, *24*, C9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butane; C_4H_{10}; [106-97-8] (2) Deuterium oxide (heavy water); D_2O; [7789-20-0]	Ben-Naim, A.; Wilf, J.; Yaacobi, M. *J. Phys. Chem.* 1973, *77*, 95-102.

VARIABLES:	PREPARED BY:
T/K: 278.15-298.15 P/kPa: 101.325	W. Hayduk

EXPERIMENTAL VALUES:

$t^1/°C$	T^2/K	Ostwald Coefficient[1] L/cm^3cm^{-3}	Bunsen Coefficient[2] $\alpha/cm^3(STP)cm^{-3}$	Mole Fraction[2] $/10^5x_1$
5	278.15	0.0689	0.0675	5.70
10	283.15	0.0539	0.0517	4.36
15	288.15	0.0430	0.0404	3.41
20	293.15	0.0350	0.0323	2.73
25	298.15	0.0289	0.0262	2.21

[1]Original data.

[2]Calculated by compiler using real gas molar volumes.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method of Ben-Naim and Baer (1) was modified to include the use of Teflon stopcocks. Degassed liquid initially in a volumetric container was forced by a stirrer-created vortex up side-arms and through tubes containing the gas, which was saturated with vapor. The gas uptake at constant pressure was determined by means of a buret.	1. Matheson Co. Minimum specified 99.95%. 2. Darmstadt Co. Minimum sepcified purity 99.95%.

	ESTIMATED ERROR:
	$\delta L/L = 0.01$ (compiler)

	REFERENCES:
	1. Ben-Naim, A.; Baer, S. *Trans. Faraday Soc.* 1963, *59*, 2735-2741.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butane; C_4H_{10}; [106-97-8] (2) Water-d_2; D_2O; [7789-20-0]	Kresheck, G. C.; Schneider, H.; Scheraga, H. A. *J. Phys. Chem.* 1965, *69*, 3132-44.
VARIABLES: T/K = 277.15 - 328.15 p_1/kPa = 101.325	PREPARED BY: H. L. Clever

EXPERIMENTAL VALUES:

Temperature		Mol Fraction[a]				Molarity	Molality
$t/^0C$	T/K		10^5x_1			10^3c_1/mol dm^{-3}	10^3m_1/mol kg^{-1}
4	277.15	6.267,	6.236,	6.196			
	277.15[b]		6.25 ± 0.03			3.44 ± 0.02	3.12 ± 0.02
7	280.15			5.280			
10	283.15	4.528,	4.497				
15	288.15	3.531,	3.490,	3.544			
20	293.15	2.815					
25	298.15	2.359,	2.318,	2.362			
	298.15[b]		2.35 ± 0.02			1.29 ± 0.01	1.17 ± 0.01
30	303.15	1.984,		1.980			
35	308.15	1.708,	1.683				
40	313.15	1.495,		1.506			
45	318.15	1.322,	1.322				
50	323.15	1.204,	1.211				
	323.15[b]		1.21 ± 0.01			0.66 ± 0.01	0.63 ± 0.01
55	328.15			1.099			

[a] The experimental values of the mole fraction solubility were provided by H. Schneider. The last digit in each number is not significant.

[b] Smoothed values from the original paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A known quantity of the gas was introduced from a gas buret into a calibrated volume which contained a weighed quantity of water. The water was stirred until equilibrium was attained (3 to 4 hours). The amount of gas in the vapor phase at equilibrium was determined from the partial pressure of the butane and the volume of the vapor space. The volume was the difference in the empty vessel volume and the water volume. The amount of dissolved gas was obtained by difference.

The D_2O density values used were based on literature data (1). The gas volume was corrected for non-ideal behavior by use of a compressibility factor (2). At each temperature the solubility was measured at one to three partial pressures which ranged from 0.5 to 0.7 atm at 4 ^{0}C and 1.2 to 1.6 atm at 50 ^{0}C. All solubility values were normalized to a butane partial pressure of one atm.

SOURCE AND PURITY OF MATERIALS:
(1) Butane. Matheson Co., Inc. 99.94 mol per cent.

(2) Water-d_2. US Atomic Energy Commission. 99.7 mol per cent D_2O.

ESTIMATED ERROR:

$\delta x_1/x_1$ = ± 0.005

REFERENCES:
1. Steckel, F.; Szapiro, S.
   Trans. Faraday Soc. 1963, *59*, 331.

2. Silberberg, I. H.; Kuo, P. K.; McKetta, J. J.
   Petrol. Engr. 1954, *24*, 9C.