COMPONENTS:

1. Methan-d_3-amine; CH_3D_2N; [5581-55-5]
   Methanamine-d_2; CH_3D_2N; [2614-35-9]
   Methanamine-d_5; CD_5N; [3767-37-1]
   Ethanamine-d_2; $C_2H_5D_2N$; [5852-45-0]
   N-Methylmethanamine-d; C_2H_6DN; [917-72-6]
   N-(Methyl-d_3)-methan-d_3-amine; C_2HD_6N; [14802-36-9]
   N-(Methyl-d_3)-methan-d_3-amine-d; C_2D_7N; [22024-52-8]
   1-Propanamine-d_2; $C_3H_7ND_2$; [25837-80-3]
   2-Propanamine-d_2; $C_3H_7ND_2$; [7395-10-0]

2. Organic liquids

EVALUATOR:

P. G. T. Fogg,
School of Chemistry,
Polytechnic of North London,
Holloway,
London N7 8DB,
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October 1983

CRITICAL EVALUATION:

The variation of total vapor pressure with variation of concentration has been measured by Wolff *et al.* (1-6) for solutions of deuterated methanamines, propanamines, *N*-deuterated ethanamine and deuterated *N*-methylmethanamines in hexane. In addition measurements have been made on *N*-deuterated ethanamine in butane and on *N*-deuterated methanamine in *N*,*N*-dimethylmethanamine. In each case the variation of partial pressure of either component with variation of composition may be calculated and compared with values for the system containing the corresponding non-deuterated amine, also studied by Wolff *et al.*

The relative solubilities of a deuterated and a corresponding non-deuterated amine in the same solvent depent upon the temperature and the partial pressure. Differences may be up to about 10%. Differences have been discussed by Wolff *et al.* in terms of relative partial pressures at the same mole fraction concentration.

On the basis of the systems which have been studied it appears that, at all concentrations, amines which have deuterium atoms substituted into methyl groups are more volatile than the corresponding unsubstituted amines under the same conditions. At low concentrations most of the amines studied which have deuterium atoms substituted on the nitrogen atom are also more volatile than the corresponding amines containing =NH or $-NH_2$ groups. However this does not hold for the 1- and 2-propanamines. It follows that, at the same partial pressure and temperature, the deuterated compound may be less soluble than the corresponding non-deuterated compound. Wolff *et al.* showed that differences may be due to changes in vibrational frequencies causing changes in partition functions governing the distribution between condensed and gaseous state.

Increase in concentration causes the partial pressure of a *N*-deuterated amine to decrease relative to that of the corresponding *N*-hydrogen compound. The effect is more marked the lower the temperature and may lead to the *N*-deuterated compound having the greater solubility at the same partial pressure and temperature. Wolff *et al.* considered that this was due to *N*-deuterated amines having a greater tendency to associate in the liquid phase than the corresponding *N*-hydrogen compounds because bonding by deuterium atoms is stronger than hydrogen bonding. It was pointed out that effects due to association are likely to be enhanced with decrease in temperature and increase in concentration.

There appears to be no investigations of phase equilibria in deuterated amine systems by other workers for comparison with the work of Wolff *et al.* However, in the opinion of the evaluator, this work is self-consistent and of high standard and should be accepted as reliable.

References

1. Wolff, H.; Höpfner, A.
Ber. Bunsenges. Phys. Chem. 1965, *69*, 710-716.
2. Wolff, H.; Höpfner, A.
Ber. Bunsenges. Phys. Chem. 1967, *71*, 461-466.
3. Wolff, H.; Hoppel, H.-E.
Ber. Bunsenges. Phys. Chem. 1966, *70*, 874-883.
4. Wolff, H.; Würtz, R.
Ber. Bunsenges. Phys. Chem. 1968, *72*, 101-109.
5. Wolff, H.; Würtz, R.
Z. Phys. Chem. (Frankfurt am Main) 1969, *67*, 115-121.
6. Wolff, H.; Shadiakhy, A.
Fluid Phase Equilibria 1983, *11*, 267-287.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Methan-d_3-amine; CH_2D_3N; [5581-55-5] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H.; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1967, *71*, 461-466.
VARIABLES:	PREPARED BY:
Composition, temperature	P. G. T. Fogg

EXPERIMENTAL VALUES:

Variation of the total vapor pressure/Torr with variation of temperature and of mole fraction of CH_2D_3N in the liquid phase, $x_{CH_2D_3N}$

	T/K				
$x_{CH_2D_3N}$	218.15	233.15	253.15	273.15	293.15
0	1.4	3.8	14.1	45.2	120.8
0.00905	7.9	16.0	39.1	90.1	192.8
0.0187	13.8	27.7	64.5	135.3	267.1
0.0392	23.5	48.6	110.7	223.3	414.7
0.0725	32.2	71.3	170.2	343.9	627.5
0.1023	37.0	85.0	209.4	433.3	793.7
0.128	39.5	93.2	235.8	497.0	919.0
0.145	40.6	97.3	250.6	532.6	990.2
0.185	42.1	104.4	278.6	607.6	1150.9
0.216	43.2	108.3	294.6	653.3	1253.2
0.263	44.2	112.5	313.1	704.8	1372.2
0.305	45.0	115.2	324.4	746.4	1464.5
0.340	45.1	116.9	333.8	774.4	1538.8
0.379	45.2	118.1	341.4	800.6	1611.6
0.419	45.5	119.5	347.5	824.3	1677.2
0.455	45.7	120.2	352.5	841.7	1728.6
0.488	45.9	120.7	356.5	856.7	1771.3
0.517	45.9	121.4	358.9	868.0	1804.9

Cont.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus described previously was used (1). Liquid mixtures of accurately known composition were introduced into a cell held in a thermostat controlled to ± 0.02°C. The total pressure was measured by a mercury manometer.

The authors calculated activity coefficients of each component by a method described by Barker (2). Constants for Redlich-Kister (3) equations for activity coefficients were evaluated and reported.

SOURCE AND PURITY OF MATERIALS:

1. CD_3NH_3Cl from Merck was treated with KOH and gave CD_3NH_2 which was purified by repeated fractionation as for CH_3ND_2 (4).
2. Supplied by Fluka; purity 99.96 mol %.

ESTIMATED ERROR:

$\delta T/K = \pm 0.02$ (estimated by authors)

REFERENCES:

1. Wolff, H; Höpfner, A. *Z. Elektrochem.* 1962, *66*, 149.
2. Barker, J.A. *Aust. J. Chem.* 1953, *6*, 207.
3. Redlich, O.; Kister, A.T. *Ind. Eng. Chem.* 1948, *21*, 345.
4. Wolff, H.; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1965, *69*, 710.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Methan-d_3-amine; CH_2D_3N; [5581-55-5] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H.; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1967, *71*, 461-466.
VARIABLES: Composition, temperature	PREPARED BY: P. G. T. Fogg

EXPERIMENTAL VALUES: Cont.

$x_{CH_2D_3N}$	218.15	233.15	253.15	273.15	293.15
0.540	46.2	121.6	360.9	876.8	1829.2
0.571	45.6	121.6	363.6	887.1	1861.6
0.601	45.9	121.9	366.4	896.1	1889.5
0.623	45.7	122.4	367.7	902.7	1909.6
0.641	45.7	122.5	368.5	906.3	1917.8
0.709	45.9	123.4	373.5	925.8	1979.0
0.715	45.8	122.9	373.8	927.9	1986.5
0.785	45.7	124.4	379.3	946.4	2039.6
0.853	46.0	125.3	384.8	966.8	2095.0
0.897	46.1	126.4	389.4	982.0	2132.4
0.946	47.0	128.4	396.2	1003.0	2186.5
1	48.0	131.5	407.4	1033.3	2256.4

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Methan-d_3-amine; CH_2D_3N; [5581-55-5]	Wolff, H.; Höpfner, A.
2. Hexane; C_6H_{14}; [110-54-3]	*Ber. Bunsenges. Phys. Chem.* 1967, *71*, 461-466.

EXPERIMENTAL VALUES:

Constants for calculation of activity coefficients from the Redlich-Kister equations given below

T/K	A	B	C	D	E
218.15	2.385	0.094	0.421	-0.012	0.106
223.15	2.338	0.107	0.413	+0.072	0.136
233.15	2.208	0.121	0.351	+0.074	0.080
243.15	2.087	0.147	0.301	+0.093	0.069
253.15	1.959	0.165	0.268	+0.094	0.043
263.15	1.832	0.179	0.231	+0.090	0.027
273.15	1.708	0.191	0.206	+0.080	0.006
283.15	1.585	0.200	0.188	+0.074	-0.006
293.15	1.467	0.203	0.179	+0.067	-0.022

$$\ln f_1 = A x_2^2 - B x_2^2(1 - 4 x_1) + C x_2^2(1 - 8 x_1 + 12 x_1^2) - D x_2^2(1 - 12 x_1 + 36 x_1^2 - 32 x_1^3) + E x_2^2(1 - 16 x_1 + 72 x_1^2 - 128 x_1^3 + 80 x_1^4)$$

$$\ln f_2 = A x_1^2 + B x_1^2(1 - 4 x_2) + C x_1^2(1 - 8 x_2 + 12 x_2^2) + D x_1^2(1 - 12 x_2 + 36 x_2^2 - 32 x_2^3) + E x_1^2(1 - 16 x_2 + 72 x_2^2 - 128 x_2^3 + 80 x_2^4)$$

where f_1 = activity coefficient of methan-d_3-amine
f_2 = activity coefficient of hexane
x_1 = mole fraction of methan-d_3-amine in the liquid phase
x_2 = mole fraction of hexane in the liquid phase

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Methanamine-d_2; CH_3D_2N; [2614-35-9] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H.; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1965, *69*, 710-716.
VARIABLES:	PREPARED BY:
Composition, temperature	P. G. T. Fogg

EXPERIMENTAL VALUES:

Variation of the total vapor pressure/Torr with variation of temperature and of mole fraction of CH_3D_2N in the liquid phase, $x_{CH_3D_2N}$

	T/K				
$x_{CH_3D_2N}$	218.15	233.15	253.15	273.15	293.15
0	1.0	3.7	14.3	45.4	121.0
0.0107	8.7	17.8	43.1	96.9	204.0
0.0202	14.2	28.9	66.8	140.3	275.1
0.0364	21.1	44.1	102.2	207.5	388.6
0.0465	24.3	52.4	122.4	247.2	458.0
0.0600	27.3	60.8	144.7	294.1	540.7
0.0706	29.6	66.7	161.3	330.6	606.3
0.0926	32.6	75.9	189.8	393.3	724.7
0.1134	34.3	82.4	211.7	447.7	830.1
0.145	36.3	89.3	237.3	513.2	965.9
0.176	37.6	94.4	257.1	568.6	1086.2
0.214	38.6	98.6	274.2	620.5	1204.7
0.248	38.8	100.6	286.2	657.8	1292.0
0.301	39.2	103.5	300.3	704.7	1411.9
0.338	39.7	104.6	307.5	729.2	1474.9
0.390	39.8	105.9	315.9	758.9	1558.6
0.434	39.8	106.7	320.7	778.8	1613.6
0.472	39.9	107.5	324.8	794.5	1660.8

Cont.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus described previously was used (1). Liquid mixtures of accurately known composition were introduced into a cell held in a thermostat controlled to ± 0.02°C. The total vapor pressure was measured by a mercury manometer.

The authors calculated activity coefficients of each component by a method described by Barker (2). Constants for Redlich-Kister equations for activity coefficients were evaluated and reported.

SOURCE AND PURITY OF MATERIALS:

1. Prepared from CH_3NH_2 and D_2O; repeatedly fractionated until first and last fractions had vapor pressures which differed by less than 0.5 Torr at 20°C. Spectroscopic measurements indicated that the product was 98-99% pure.
2. Material of high purity; dried over P_2O_5; distilled and repeatedly fractionated until first and last fractions had the same vapor pressures as indicated by a manometer (1).

ESTIMATED ERROR:

$\delta T/K = \pm 0.02$ (estimated by authors)

REFERENCES:

1. Wolff, H; Höpfner, A. *Z. Elektrochem.* 1962, *66*, 149.
2. Barker, J.A. *Aust. J. Chem.* 1953, *6*, 207.
3. Redlich, O.; Kister, A.T. *Ind. Eng. Chem.* 1948, *21*, 345.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Methanamine-d_2; CH_3D_2N; [2614-35-9] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H.; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1965, *69*, 710-716.
VARIABLES: Composition, temperature	PREPARED BY: P. G. T. Fogg

EXPERIMENTAL VALUES: Cont.

	T/K				
$x_{CH_3D_2N}$	218.15	233.15	253.15	273.15	293.15
0.535	40.0	108.3	329.9	815.6	1727.1
0.567	39.9	108.5	331.8	824.1	1753.0
0.629	40.3	109.1	336.0	840.7	1805.6
0.680	40.2	109.4	339.0	853.3	1842.6
0.730	40.0	110.4	341.2	864.5	1876.5
0.802	40.3	110.6	346.3	881.6	1928.3
0.872	40.1	111.4	351.0	899.7	1980.7
0.918	40.4	112.5	355.9	915.2	2021.5
0.957	41.1	114.0	361.0	930.7	2059.4
0.972	41.2	114.5	363.5	937.6	2074.8
1	41.4	116.1	368.7	950.2	2107.7

Constants for calculation of activity coefficients from the Redlich-Kister equations given below

T/K	A	B	C
218.15	2.460	0.141	0.601
223.15	2.377	0.110	0.508
228.15	2.320	0.124	0.458
233.15	2.252	0.122	0.405
243.15	2.135	0.148	0.325
253.15	2.008	0.166	0.269
263.15	1.884	0.185	0.221
273.15	1.764	0.201	0.190
283.15	1.640	0.207	0.163
293.15	1.519	0.211	0.142

$$\ln f_1 = A x_2^2 - B x_2^2(1 - 4 x_1) + C x_2^2(1 - 8 x_1 + 12 x_1^2)$$

$$\ln f_2 = A x_1^2 + B x_1^2(1 - 4 x_2) + C x_1^2(1 - 8 x_2 + 12 x_2^2)$$

where f_1 = activity coefficient of methanamine-d_2
f_2 = activity coefficient of hexane
x_1 = mole fraction of methanamine-d_2 in the liquid phase
x_2 = mole fraction of hexane in the liquid phase

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Methanamine-d_5; CD_5N; [3767-37-1] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H.; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1967, *71*, 461-466.
VARIABLES:	PREPARED BY:
Composition, temperature	P. G. T. Fogg

EXPERIMENTAL VALUES:

Variation of the total vapor pressure/Torr with variation of temperature and of mole fraction of CD_5N in the liquid phase.

	T/K				
x_{CD_5N}	218.15	233.15	253.15	273.15	293.15
0	1.0	3.7	14.3	45.4	121.0
0.0112	9.4	19.2	45.8	101.7	211.1
0.0221	15.7	32.1	73.6	152.7	295.4
0.0329	20.6	42.8	98.5	199.7	373.6
0.0434	24.3	51.9	119.8	242.2	447.3
0.0538	27.2	59.2	139.5	281.7	516.3
0.0639	29.8	65.6	156.2	317.3	579.6
0.0737	31.4	70.7	171.4	350.1	638.8
0.0878	33.7	77.1	190.4	392.7	719.5
0.1016	35.0	82.2	206.9	431.1	792.6
0.114	36.3	86.2	219.4	462.1	854.2
0.154	38.6	94.9	252.2	547.7	1032.0
0.191	40.0	100.3	274.1	609.4	1167.6
0.238	40.9	105.0	294.4	668.8	1306.7
0.239	40.9	105.1	294.7	670.1	1311.2
0.274	41.0	107.2	304.7	702.5	1386.7
0.308	41.6	108.5	313.0	732.5	1463.7
0.336	41.2	109.2	318.8	753.3	1519.0
0.393	41.6	110.7	327.5	785.4	1609.9

Cont.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus described previously was used (1). Liquid mixtures of accurately known composition were introduced into a cell held in a thermostat controlled to ± 0.02°C. The total vapor pressure was measured by a mercury manometer.

The authors calculated activity coefficients of each component by a method described by Barker (2). Constants for Redlich-Kister(3) equations for activity coefficients were evaluated and reported.

SOURCE AND PURITY OF MATERIALS:

1. CD_3NH_3Cl from Merck was treated with KOH to give CD_3NH_2 which was then allowed to react with D_2O to give CD_3ND_2. Purification by repeated fractionation as for CH_3ND_2 (4).
2. Supplied by FLUKA A.G.;purity 99.96 mol %.

ESTIMATED ERROR:

$\delta T/K = \pm 0.02$ (authors' estimate)

REFERENCES:

1. Wolff, H.; Höpfner, A. *Z. Elektrochem.* 1962, *66*, 149.
2. Barker, J.A. *Aust. J. Chem.* 1953, *6*, 207.
3. Redlich, O.; Kister, A.T. *Ind. Eng. Chem.* 1948, *21*, 345.
4. Wolff, H.; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1965, *69*, 710.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Methanamine-d_5; CD_5N; [3767-37-1] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1967, *71*, 461-466.
VARIABLES:	PREPARED BY:
Composition, temperature	P. G. T. Fogg

EXPERIMENTAL VALUES: Cont.

	T/K				
x_{CD_5N}	218.15	233.15	253.15	273.15	293.15
0.436	41.0	111.0	332.8	806.1	1666.0
0.452	41.6	111.8	334.5	812.5	1684.9
0.479	41.2	111.8	337.3	823.0	1717.0
0.522	41.2	112.5	341.4	838.3	1764.6
0.561	41.5	112.7	343.7	849.7	1801.6
0.613	41.6	113.0	346.7	863.7	1841.6
0.663	41.7	113.5	349.3	877.0	1885.4
0.717	41.7	114.3	353.0	889.3	1922.0
0.786	41.8	114.4	357.0	905.4	1973.4
0.838	41.6	115.0	360.6	919.0	2011.6
0.910	42.3	116.5	367.3	942.4	2075.1
0.942	42.6	118.0	371.6	954.3	2105.5
0.979	42.9	119.4	377.5	972.0	2146.3
1	43.2	120.2	380.4	981.6	2170.4

760 Torr = 1 atm = 1.013×10^5 Pa.

Constants for calculation of activity coefficients from the Redlich-Kister equations given below.

T/K	A	B	C	D	E
218.15	2.456	0.050	0.445	0.140	0.275
223.15	2.399	0.089	0.436	0.087	0.177
233.15	2.272	0.106	0.372	0.100	0.123
243.15	2.141	0.134	0.329	0.092	0.071
253.15	2.018	0.157	0.290	0.107	0.054
263.15	1.886	0.170	0.245	0.099	0.030
273.15	1.763	0.184	0.212	0.096	0.024
283.15	1.639	0.196	0.192	0.093	0.010
293.15	1.519	0.195	0.163	0.091	0.011

$$\ln f_1 = A x_2^2 - B x_2^2(1 - 4 x_1) + C x_2^2(1 - 8 x_1 + 12 x_1^2) - D x_2^2(1 - 12 x_1 + 36 x_1^2 - 32 x_1^3) + E x_2^2(1 - 16 x_1 + 72 x_1^2 - 128 x_1^3 + 80 x_1^4)$$

$$\ln f_2 = A x_1^2 + B x_1^2(1 - 4 x_2) + C x_1^2(1 - 8 x_2 + 12 x_2^2) + D x_1^2(1 - 12 x_2 + 36 x_2^2 - 32 x_2^3) + E x_1^2(1 - 16 x_2 + 72 x_2^2 - 128 x_2^3 + 80 x_2^4)$$

where f_1 = activity coefficient of methanamine-d_5

f_2 = activity coefficient of hexane

x_1 = mole fraction of methanamine-d_5 in the liquid phase

x_2 = mole fraction of hexane in the liquid phase.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethanamine-d_2; $C_2H_5D_2N$; [5852-45-9] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff,H.; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1965, *69*, 710-716.
VARIABLES:	PREPARED BY:
Composition, Temperature	P. G. T. Fogg

EXPERIMENTAL VALUES:

Variation of the total vapor pressure/Torr with variation of temperature and of mole fraction of $C_2H_5D_2N$ in the liquid phase, $x_{C_2H_5D_2N}$

	T/K			
$x_{C_2H_5D_2N}$	233.15	253.15	273.15	293.15
0	3.9	14.6	45.9	121.1
0.0176	8.0	25.0	67.9	162.4
0.0329	11.0	33.0	85.5	196.0
0.0452	12.9	38.9	98.6	221.4
0.0891	18.2	55.1	138.3	301.9
0.1165	20.0	62.7	158.2	344.7
0.2095	24.6	79.4	207.2	458.1
0.239	25.0	83.4	218.2	486.3
0.305	26.7	88.9	239.9	540.6
0.339	28.1	93.4	249.7	564.6
0.362	27.6	94.0	254.6	577.3
0.409	28.3	97.2	264.1	604.9
0.455	28.9	99.7	273.5	629.3
0.468	29.2	100.5	275.8	636.4
0.517	29.6	102.9	284.1	659.5
0.582	30.1	105.9	294.0	686.2
0.617	30.7	107.5	299.7	701.3
0.683	31.0	110.1	307.5	725.8
0.723	31.7	112.1	314.1	741.8

Cont.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus described previously was used (1). Liquid mixtures of accurately known composition were introduced into a cell held in a thermostat controlled to ± 0.02°C. The total vapor pressure was measured by a mercury manometer.

The authors calculated activity coefficients of each component by a method described by Barker (2). Constants for Redlich-Kister equations for activity coefficients were evaluated and reported.

SOURCE AND PURITY OF MATERIALS:

1. Prepared from $C_2H_5NH_2$ and D_2O; repeatedly fractionated until first and last fractions had vapor pressures which differed by 0.4 Torr at 20°C. Spectroscopic measurements indicated that the product was at least 99% pure.
2. Material of high purity; dried over P_2O_5; distilled and repeatedly fractionated until first and last fractions had the same vapor pressures as indicated by a manometer (1).

ESTIMATED ERROR:

δT/K = ± 0.02 (estimated by authors)

REFERENCES:

1. Wolff, H.; Höpfner, A. *Z. Elektrochem.* 1962, *66*, 149.
2. Barker, J.A. *Aust. J. Chem.* 1953, *6*, 207.
3. Redlich, O.; Kister, A.T. *Ind. Eng. Chem.* 1948, *21*, 345.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethanamine-d_2; $C_2H_5D_2N$; [5852-45-9] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff,H.; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1965, *69*, 710-716.
VARIABLES:	PREPARED BY:
Composition, Temperature	P. G. T. Fogg

EXPERIMENTAL VALUES: Cont.

	T/K			
$x_{C_2H_5D_2N}$	233.15	253.15	273.15	293.15
0.793	32.1	114.7	323.9	767.0
0.832	32.5	116.5	329.6	782.8
0.898	33.7	119.6	339.2	806.9
0.987	34.9	123.9	352.2	841.3
1	34.8	124.5	354.7	847.2

760 Torr = 1 atm = 1.013×10^5 Pa

Constants for calculation of activity coefficients from the Redlich-Kister equations given below

T/K	A	B	C
233.15	1.728	-0.078	0.191
243.15	1.630	-0.036	0.174
253.15	1.535	+0.001	0.148
263.15	1.434	+0.017	0.109
273.15	1.332	+0.037	0.087
283.15	1.237	+0.048	0.066
293.15	1.145	+0.061	0.063

$$\ln f_1 = A x_2^2 - B x_2^2(1 - 4 x_1) + C x_2^2(1 - 8 x_1 + 12 x_1^2)$$

$$\ln f_2 = A x_1^2 + B x_1^2(1 - 4 x_2) + C x_1^2(1 - 8 x_2 + 12 x_2^2)$$

where f_1 = activity coefficient of ethanamine -d_2

f_2 = activity coefficient of hexane

x_1 = mole fraction of ethanamine-d_2 in the liquid phase

x_2 = mole fraction of hexane in the liquid phase.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. *N*-Methyl-methanamine-d; C_2H_6DN; [917-72-6] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H.; Würtz, R. *J. Phys. Chem.* 1970, *74*, 1600-1606.
VARIABLES:	PREPARED BY:
Composition, temperature	P. G. T. Fogg

EXPERIMENTAL VALUES:

Variation of the total vapor pressure/Torr with variation of temperature and of mole fraction of C_2H_6DN in the liquid phase, $x_{C_2H_6DN}$

	T/K							
$x_{C_2H_6DN}$	223.15	233.15	243.15	253.15	263.15	273.15	283.15	293.15
0	2.2	3.8	7.7	14.3	26.7	45.5	75.6	121.1
0.0048	2.5	5.0	9.4	17.3	30.8	52.4	85.2	133.4
0.0075	3.0	5.7	10.8	19.7	33.8	56.6	91.0	141.3
0.0207	4.9	9.0	15.3	27.9	45.3	74.1	114.8	173.2
0.0254	5.6	10.0	18.0	30.5	50.4	79.9	122.7	183.6
0.0484	8.2	15.2	26.6	44.3	70.6	108.9	163.2	238.6
0.0705	10.2	18.9	33.3	55.0	87.4	133.6	198.3	286.4
0.0922	11.8	22.5	39.1	64.7	102.3	156.3	231.1	331.8
0.1541	15.2	28.9	51.7	86.6	137.5	209.8	307.9	437.8
0.2535	18.3	35.7	64.9	111.3	178.2	276.6	409.5	584.6
0.3053	19.1	37.7	69.6	119.8	194.5	301.9	448.8	642.3
0.3526	20.1	40.1	73.9	128.3	209.5	327.1	484.9	706.3
0.4109	20.9	41.8	78.2	135.5	223.0	350.7	527.6	765.1
0.4494	21.5	43.2	80.2	140.4	231.1	364.3	549.6	798.5
0.5077	22.2	44.6	83.6	147.1	243.4	384.6	582.0	846.3
0.6055	23.1	47.3	88.8	157.3	262.1	417.3	635.5	932.2
0.6554	23.8	48.4	91.6	162.0	268.6	432.1	659.8	970.1
0.7038	24.6	49.7	94.0	167.3	279.5	447.4	685.0	1009.4
0.7538	25.0	50.9	96.7	172.2	288.2	461.5	708.6	1046.4

Cont.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus described previously was used (1). Liquid mixtures of accurately known composition were introduced into a cell held in a thermostat controlled to ± 0.02°C. The total vapor pressure was measured by a mercury manometer.

The authors calculated activity coefficients of each component from the vapor pressure data by a method described by Barker (2). Constants for Redlich-Kister equations for activity coefficients were evaluated and reported.

SOURCE AND PURITY OF MATERIALS:

1. Prepared from dimethylammonium chloride; repeatedly fractionated until first and last fractions had vapor pressures within 0.2 Torr.
2. Research grade (Phillips Petroleum Co., Bartlesville, Oklahoma).

ESTIMATED ERROR:

δT/K = ± 0.02 (estimated by authors)

REFERENCES:

1. Wolff, H.; Höpfner, A. *Z. Elektrochem.* 1962, *66*, 149.
2. Barker, J.A. *Aust. J. Chem.* 1953 *6*, 207.
3. Redlich, O.; Kister, A.T. *Ind. Eng Chem.* 1948, *21*, 345.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. *N*-Methyl-methanamine-d; C_2H_6DN; [917-72-6] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H.; Würtz, R. *J. Phys. Chem.* 1970, *74*, 1600-1606.
VARIABLES:	PREPARED BY:
Composition, temperature	P. G. T. Fogg

EXPERIMENTAL VALUES: Cont.

	T/K							
$x_{C_2H_6DN}$	223.15	233.15	243.15	253.15	263.15	273.15	283.15	293.15
0.8037	25.7	52.5	100.5	177.3	297.6	477.2	734.1	1086.1
0.8545	26.6	54.2	102.4	182.6	307.2	493.1	759.0	1125.1
0.9021	27.3	55.6	105.7	188.3	316.8	509.3	784.9	1164.8
1	28.8	58.9	112.2	201.0	338.4	545.1	841.1	1249.2

760 Torr = 1 atm = 1.013×10^5 Pa.

Constants for calculation of activity coefficients from the Redlich-Kister equations given below.

T/K	A	B	C
223.15	1.482	-0.081	0.119
233.15	1.431	-0.029	0.139
243.15	1.326	+0.002	0.111
253.15	1.225	+0.016	0.090
263.15	1.113	+0.033	0.066
273.15	1.021	+0.047	0.066
283.15	0.920	+0.053	0.068
293.15	0.828	+0.057	0.061

$$\ln f_1 = A x_2^2 - B x_2^2(1 - 4 x_1) + C x_2^2(1 - 8 x_1 + 12 x_1^2)$$

$$\ln f_2 = A x_1^2 + B x_1^2(1 - 4 x_2) + C x_1^2(1 - 8 x_2 + 12 x_2^2)$$

where f_1 = activity coefficient of the amine
f_2 = activity coefficient of hexane
x_1 = mole fraction of the amine in the liquid phase
x_2 = mole fraction of hexane in the liquid phase

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. *N*-(methyl-d_3)-methan-d_3-amine; C_2HD_6N; [14802-36-9] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H.; Würtz, R. *J. Phys. Chem.* 1970, *74*, 1600-1606.
VARIABLES:	PREPARED BY:
Composition, temperature	P. G. T. Fogg

EXPERIMENTAL VALUES:

Variation of the total vapor pressure/Torr with variation of temperature and of mole fraction of C_2HD_6N in the liquid phase, $x_{C_2HD_6N}$

	T/K							
$x_{C_2HD_6N}$	223.15	233.15	243.15	253.15	263.15	273.15	283.15	293.15
0	2.2	3.8	7.7	14.3	26.7	45.5	75.6	121.1
0.0103	3.5	6.7	12.1	21.6	36.7	60.4	96.0	148.5
0.0254	5.8	10.5	18.6	31.4	51.2	81.9	124.7	185.9
0.0509	8.9	16.4	28.2	46.4	73.9	113.6	169.9	247.1
0.0763	11.5	20.9	36.4	59.8	94.4	143.9	212.1	304.1
0.1016	13.6	25.1	43.3	71.7	112.3	170.9	250.9	357.6
0.1504	16.2	30.6	54.0	90.3	141.8	214.7	312.9	442.5
0.2525	20.1	38.8	70.1	118.8	190.2	291.1	428.5	609.1
0.2685	20.3	39.8	72.2	122.0	195.3	299.3	441.2	626.0
0.2778	20.8	40.2	73.0	123.8	198.7	305.5	449.7	638.5
0.3539	22.6	44.1	80.7	138.5	223.8	347.5	516.1	739.9
0.4063	23.4	46.1	84.5	146.0	237.7	370.4	553.2	795.8
0.4258	23.7	46.8	86.5	149.4	243.9	380.2	569.3	819.9
0.5014	24.8	49.5	91.5	159.5	260.9	409.4	615.2	891.3
0.5529	25.4	50.9	94.8	167.3	272.1	428.2	646.3	938.3
0.6053	26.9	52.3	97.8	172.2	283.4	447.9	677.9	987.1
0.6531	27.0	53.9	100.9	177.1	292.8	463.9	703.8	1029.4
0.7044	28.5	55.3	103.8	182.5	303.3	480.9	732.0	1072.5

Cont.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus described previously was used (1). Liquid mixtures of accurately known composition were introduced into a cell held in a thermostat controlled to ± 0.02°C. The total vapor pressure was measured by a mercury manometer.

The authors calculated activity coefficients of each component from the vapor pressure data by a method described by Barker (2). Constants for Redlich-Kister equations for activity coefficients were evaluated and reported.

SOURCE AND PURITY OF MATERIALS:

1. Prepared from $(CD_3)_2NH_2Cl$ (Merck, Darmstadt); purified by repeated fractionation until first and last fractions differed in vapor pressures by less than 0.2 Torr.
2. Research grade (Phillips Petroleum Co., Bartlesville, Oklahoma.)

ESTIMATED ERROR:

$\delta T/K = \pm 0.02$ (estimated by authors)

REFERENCES:

1. Wolff, H.; Höpfner, A. *Z. Elektrochem.* 1962, *66*, 149.
2. Barker, J.A. *Aust. J. Chem.* 1953, *6*, 207.
3. Redlich, O.; Kister, A.T. *Ind. Eng. Chem.* 1948, *21*, 345.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. *N*-(methyl-d_3)-methan-d_3-amine; C_2HD_6N; [14802-36-9] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H.; Würtz, R. *J. Phys. Chem.* 1970, *74*, 1600-1606.
VARIABLES:	PREPARED BY:
Composition, temperature	P. G. T. Fogg

EXPERIMENTAL VALUES: Cont.

	T/K							
$x_{C_2HD_6N}$	223.15	233.15	243.15	253.15	263.15	273.15	283.15	293.15
0.7546	28.6	56.9	106.8	188.1	312.9	497.9	759.1	1114.5
0.8024	29.3	58.2	109.7	193.9	322.7	514.4	785.0	1156.3
0.8529	29.9	60.1	113.1	200.1	333.5	531.8	813.5	1198.5
0.9218	31.2	63.0	118.4	209.2	349.8	558.7	855.0	1262.2
1	32.8	66.0	124.8	221.1	369.8	591.5	906.6	1339.4

760 Torr = 1 atm = 1.013×10^5 Pa

Constants for calculation of activity coefficients from the Redlich-Kister equations given below

T/K	A	B	C
223.15	1.452	-0.029	0.168
233.15	1.396	-0.010	0.121
243.15	1.287	+0.014	0.086
253.15	1.189	+0.033	0.076
263.15	1.078	+0.047	0.056
273.15	0.984	+0.054	0.054
283.15	0.888	+0.061	0.049
293.15	0.792	+0.063	0.049

$$\ln f_1 = A x_2^2 - B x_2^2(1 - 4 x_1) + C x_2^2(1 - 8 x_1 + 12 x_1^2)$$

$$\ln f_2 = A x_1^2 + B x_1^2(1 - 4 x_2) + C x_1^2(1 - 8 x_2 + 12 x_2^2)$$

where f_1 = activity coefficient of the amine
f_2 = activity coefficient of hexane
x_1 = mole fraction of the amine in the liquid phase
x_2 = mole fraction of hexane in the liquid phase

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. *N*-(methyl-d_3)-methan-d_3-amine-d; C_2D_7N; [22024-52-8] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H.; Würtz, R. *J. Phys. Chem.* 1970, *74*, 1600-1606.
VARIABLES:	PREPARED BY:
Composition, temperature	P. G. T. Fogg

EXPERIMENTAL VALUES:

Variation of the total vapor pressure/Torr with variation of temperature and of mole fraction of C_2D_7N in the liquid phase, $x_{C_2D_7N}$

	T/K							
$x_{C_2D_7N}$	223.15	233.15	243.15	253.15	263.15	273.15	283.15	293.15
0	2.2	3.8	7.7	14.3	26.7	45.5	75.6	121.1
0.0103	3.1	6.5	12.7	21.6	36.9	60.7	96.5	148.6
0.0256	5.9	10.4	18.7	31.8	51.9	82.1	125.7	187.6
0.0503	8.9	16.1	28.0	46.6	73.9	114.1	170.5	247.5
0.0761	11.6	21.1	36.2	60.0	94.6	144.3	212.7	305.8
0.1012	13.0	24.4	42.9	71.4	112.5	171.3	251.8	359.7
0.1516	15.9	30.4	53.9	90.3	142.9	218.0	320.3	456.3
0.2028	18.4	34.9	62.3	104.7	166.7	254.9	374.0	528.9
0.2538	19.8	37.9	68.7	117.0	187.6	288.6	426.0	605.5
0.3003	20.1	39.9	73.2	125.6	203.4	314.5	466.8	666.6
0.3512	21.4	42.2	77.8	133.7	218.0	339.6	506.8	727.3
0.4005	22.2	43.8	81.7	141.9	232.0	363.0	544.4	785.2
0.4504	22.9	45.7	84.8	148.1	242.9	381.6	572.8	827.7
0.5019	23.2	47.2	88.1	153.8	253.3	398.9	602.3	873.4
0.5485	24.1	48.5	91.1	159.8	264.6	418.1	633.7	924.4
0.6022	25.1	50.0	93.9	165.5	274.3	435.5	661.0	966.9
0.6533	25.5	51.2	96.8	171.3	284.9	453.2	690.7	1012.9
0.7011	26.0	52.8	99.6	176.0	293.4	468.0	714.2	1050.0

Cont.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus described previously was used (1). Liquid mixtures of accurately known composition were introduced into a cell held in a thermostat controlled to ± 0.02°C. The total vapor pressure was measured by a mercury manometer.

The authors calculated activity coefficients of each component from the vapor pressure data by a method described by Barker (2). Constants for Redlich-Kister equations (3) for activity coefficients were evaluated and reported.

SOURCE AND PURITY OF MATERIALS:

1. $(CD_3)_2NH_2Cl$ (Merck, Darmstadt) was used to prepare $(CD_3)_2NH$ which was then converted to $(CD_3)_2ND$ by the action of D_2O. Purification was by repeated fractionation until first and last fractions had vapor pressures within 0.2 Torr (1), (4).
2. Research grade (Phillips Petroleum Co., Bartlesville, Oklahoma.)

ESTIMATED ERROR:

$\delta T/K = \pm 0.02$ (estimated by authors)

REFERENCES:

1. Wolff, H.; Höpfner, A. *Z. Elektrochem.* 1962, *66*, 149.
2. Barker, J.A. *Aust. J. Chem.* 1953, *6*, 207.
3. Redlich, O.; Kister, A.T. *Ind. Eng. Chem.* 1948, *21*, 345.
4. Wolff, H.; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1965, *69*, 710.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. *N*-(methyl-d_3)-methan-d_3-amine-d; C_2D_7N; [22024-52-8] 2. Hexane; C_6H_{14}; [110-54-3]	Wolff, H.; Würtz, R. *J. Phys. Chem.* 1970, *74*, 1600-1606.
VARIABLES:	PREPARED BY:
Composition, temperature	P. G. T. Fogg

EXPERIMENTAL VALUES: Cont.

	T/K							
$x_{C_2D_7N}$	223.15	233.15	243.15	253.15	263.15	273.15	283.15	293.15
0.7533	26.8	54.3	102.5	181.7	303.6	484.9	741.7	1092.5
0.8003	27.4	55.6	105.5	186.7	312.5	499.7	766.3	1130.4
0.8519	28.7	57.6	108.6	192.8	323.2	517.9	795.7	1175.8
0.9012	29.4	59.3	112.0	199.0	333.4	535.5	823.0	1219.0
1	30.8	62.4	119.0	212.3	356.5	572.9	882.1	1309.7

760 Torr = 1 atm = 1.013×10^5 Pa

Constants for calculation of activity coefficients from the Redlich-Kister equations given below

T/K	A	B	C
223.15	1.495	-0.078	0.137
233.15	1.441	-0.016	0.151
243.15	1.328	+0.006	0.109
253.15	1.228	+0.021	0.097
263.15	1.117	+0.038	0.077
273.15	1.023	+0.045	0.073
283.15	0.925	+0.050	0.067
293.15	0.824	+0.046	0.063

$$\ln f_1 = A x_2^2 - B x_2^2(1 - 4 x_1) + C x_2^2(1 - 8 x_1 + 12 x_1^2)$$

$$\ln f_2 = A x_1^2 + B x_1^2(1 - 4 x_2) + C x_1^2(1 - 8 x_2 + 12 x_2^2)$$

where f_1 = activity coefficient of the amine
f_2 = activity coefficient of hexane
x_1 = mole fraction of the amine in the liquid phase
x_2 = mole fraction of hexane in the liquid phase

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Methanamine-d_2; CH_3D_2N; [2614-35-9] 2. *N,N*-Dimethylmethanamine, (trimethylamine); C_3H_9N; [75-50-3]	Wolff, H; Würtz, R. *Z. Phys. Chem. (Frankfurt am Main)* 1969, *67*, 115-121
VARIABLES: Composition, temperature	PREPARED BY: P. G. T. Fogg

EXPERIMENTAL VALUES:

Variation of the total vapor pressure/Torr with variation of temperature and of mole fraction of CH_3D_2N in the liquid phase, $x_{CH_3D_2N}$

	T/K				
$x_{CH_3D_2N}$	223.15	233.15	253.15	273.15	293.15
0	56.4	102.3	288.3	676.9	1387.0
0.0105	57.8	105.0	293.2	687.1	1411.9
0.0301	59.7	107.8	302.0	708.1	1454.3
0.0505	60.4	109.6	310.6	727.6	1495.2
0.0689	61.8	111.7	316.7	744.3	1530.6
0.0901	63.0	115.3	327.1	769.7	1582.1
0.0994	63.3	115.5	327.0	770.9	1589.0
0.1502	65.0	119.2	341.0	807.3	1665.7
0.1973	66.7	122.8	352.7	838.8	1737.0
0.2475	68.0	125.2	362.6	864.6	1798.3
0.2981	68.7	127.3	371.3	892.2	1862.5
0.3664	69.5	129.3	379.1	920.4	1928.1
0.4076	69.8	130.3	383.8	931.9	1960.1
0.4481	69.5	130.9	388.2	944.1	1991.0
0.4980	70.0	131.9	391.5	956.8	2029.8
0.5401	70.4	132.4	394.6	968.7	2053.0
0.6020	69.3	131.5	396.5	976.9	2084.1
0.6446	69.5	131.5	398.1	983.0	2107.0

Cont.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus described previously was used (1). Liquid mixtures of accurately known composition were introduced into a cell held in a thermostat controlled to ± 0.02°C. The total vapor pressure was measured by a mercury manometer.

The authors calculated activity coefficients of each component by a method described by Barker (2). Constants for Redlich-Kister equations (3) for activity coefficients were evaluated and reported.

SOURCE AND PURITY OF MATERIALS:

1. Prepared from CH_3NH_2 and D_2O; repeatedly fractionated until the first and last fractions had vapor pressures which differed by less than 0.5 torr at 20°C (4).
2. Prepared from trimethylammonium hydrochloride and purified as 1 (5).

ESTIMATED ERROR:

$\delta T/K = \pm 0.02$ (estimated by authors)

REFERENCES:
1. Wolff, H.; Höpfner, A. *Z. Elektrochem.* 1962, *66*, 149.
2. Barker, J.A. *Aust. J. Chem.* 1953, *6*, 207.
3. Redlich, O.; Kister, A.T. *Ind. Eng. Chem.* 1948, *21*, 345.
4. Wolff, H.; Höpfner, A. *Ber. Bunsenges. Phys. Chem.* 1965, *69*, 710
5. Wolff, H.; Würtz, R. *Ber. Bunsenges. Phys. Chem.* 1968, *72*, 101.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Methanamine-d_2; CH_3D_2N; [2614-35-9] 2. *N,N*-Dimethylmethanamine, (trimethylamine); C_3H_9N; [75-50-3]	Wolff, H; Würtz, R. *Z. Phys. Chem. (Frankfurt am Main)* **1969**, *67*, 115-121.
VARIABLES:	PREPARED BY:
Composition, temperature	P. G. T. Fogg

EXPERIMENTAL VALUES: Cont.

	T/K				
$x_{CH_3D_2N}$	223.15	233.15	253.15	273.15	293.15
0.7466	68.7	129.6	396.7	989.2	2137.6
0.8485	66.1	126.3	390.5	984.9	2145.6
0.8965	64.3	123.7	385.5	978.8	2143.5
0.9487	61.7	120.3	378.4	966.0	2128.3
1	59.1	115.6	367.4	947.8	2105.4

760 Torr = 1 atm = 1.013×10^5 Pa

Constants for calculation of activity coefficients from the Redlich-Kister equations given below

T/K	A	B	C
223.15	0.767	-0.075	0.139
233.15	0.749	-0.059	0.071
243.15	0.719	-0.013	0.036
253.15	0.692	0.000	0.052
263.15	0.659	+0.019	0.056
273.15	0.621	+0.028	0.028
283.15	0.578	+0.038	0.037
293.15	0.539	+0.031	0.040

$$\ln f_1 = A x_2^2 - B x_2^2(1 - 4 x_1) + C x_2^2(1 - 8 x_1 + 12 x_1^2)$$

$$\ln f_2 = A x_1^2 + B x_1^2(1 - 4 x_2) + C x_1^2(1 - 8 x_2 + 12 x_2^2)$$

where f_1 = activity coefficient of methanamine-d_2
f_2 = activity coefficient of trimethylamine
x_1 = mole fraction of methanamine-d_2
x_2 = mole fraction of trimethylamine.