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Phase equilibrium properties of binary mixtures containing 1,3-pentanediamine (or 1,5-diamino-2-methylpentane) and water at several temperatures

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ABSTRACT

The vapor pressures of (1,3-pentanediamine + water), or (1,5-diamino-2-methylpentane + water) binary mixtures, and of pure 1,3-pentanediamine or 1,5-diamino-2-methylpentane components were measured by means of a static device at temperatures between (273 and 363) K. The data were correlated with the Antoine equation. From these data excess Gibbs functions (G^E) were calculated for several constant temperatures and fitted to a three order Redlich–Kister equation using the Barker's method. The (1,3-pentanediamine + water) or (1,5-diamino-2-methylpentane + water) binary systems exhibit negative deviations in G^E for all investigated temperatures over the whole composition. Additionally, the NRTL UNIQUAC and Modified UNIFAC (Do) models have been used for the correlation or prediction of the total pressure.

1. Introduction

The major cause of global warming is anthropogenic CO_2. Its main sources are fossil fuel based power production, traffic and industries such as cement and iron industries [1].

Among various methods proposed for CO_2 capture, the chemical absorption technology is recognized as the most mature technology. But unfortunately monoamines such as monoethanolamine (MEA) solutions exhibit low CO_2 absorption capacity. Therefore, there is a need to find new solvents or better amines to improve the efficiency of acid gas scrubbing [2]. Multiamines (diamine and triamine) based CO_2 capture method could be an alternative to conventional monoamines based CO_2 capture technology due to their high CO_2 loading capacity [3].

To test the loss of the solvent at the regeneration step of the CO_2 absorption technology, there is a need of (vapor + liquid) equilibria data of the aqueous solutions of amine [1]. In this work, we report the vapor pressure data for 1,3-pentanediamine (PDA) and 1,5-diamino-2-methylpentane (DMP) and their aqueous solutions using a static apparatus at temperatures between (273.15 and 363.15) K. The present paper extends our previous studies related to various monoamine mixtures [4–9].

The NRTL, UNIQUAC and Modified UNIFAC (Do) models have been used to correlate the vapor pressures of the pure and mixed liquids.

A survey of the literature shows that there is no data available in the open literature for the investigated diamines and nor for the aqueous solutions.

2. Experimental section

2.1. Materials

The diamines were supplied by Sigma–Aldrich. Table 1 reports the purities stated by the supplier and those obtained by gas chromatography. The water content in the amines (important in the case of pure amine study), was determined by Karl Fischer method. It was less than 30 ppm. The aqueous mixtures were prepared by weighing. The water was distilled and deionised before use. The balance uncertainty is ±0.0004 g.

2.2. VLE measurements

The vapor pressure measurements for the pure components and aqueous solutions were carried out using a static device [10–13].

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The apparatus was equipped with a differential manometer from MKS, type 670, model 616A. The pressure measurement consisted of applying the vapor pressure of the sample on the measurement side of the gauge. The reference side was submitted to a permanent-dynamic pumping. The residual pressure was 10^{-4} Pa and therefore can be neglected. Temperature measurements were carried out using a copper-constantan thermocouple calibrated against a 25 Ω platinum resistance standard thermometer ($T = \pm 0.001$ K, IPTS 90) and a Leeds & Northrup bridge ($\pm 10^{-4}$ Ω). During measurements the stability of the temperature is ±0.02 K. The differential pressure gauge was calibrated against a U-manometer filled with mercury or apiezon oil depending on pressure range. The levels in both arms of the U-shaped manometer were read by a cathetometer (reference 70298, from Bouty France) to the nearest 0.001 mm. The calibration was then checked by measuring the vapor and the sublimation pressures of water and naphthalene [10]. The uncertainty of the measurements is estimated to be: $u(P/\text{Pa}) = 0.03 * P$ for $P < 600$ Pa; $u(P/\text{Pa}) = 0.01 * P$ for P in the range (600 to 1300 Pa), $u(P/\text{Pa}) = 0.003 * P$ for P over 1300 Pa, and $u(T) = 0.02$ K for the temperature range $203 \leqslant T/\text{K} \leqslant 463$. Mixtures were prepared by mass and thoroughly degassed by distillation. Once the VLE measurements were carried out, the liquid phase is recovered and the molar fraction of the components determined by gas chromatography.

3. Results and discussion

The experimental vapor pressure data were fitted to the Antoine equation [14]:

$$log_{10}P/\text{Pa} = A - \frac{B}{C + T/\text{K}}. \tag{1}$$

TABLE 1
CAS#, and purities (mass fraction) of chemicals from Sigma–Aldrich.

Component	1,3-Pentanediamine (PDA)	1,5-Diamino-2-methylpentane (DMP)
CAS #	589-37-7	15520-10-2
Supplier purity	0.98	0.99
GC Purity	>0.99	>0.99

TABLE 2
Coefficients A, B, C and overall mean relative deviation in pressure of the Antoine equation (equation (1)).

Compound	Temperature/K	A	B	C	100 ($\delta P/P$)
PDA	272.97 to 451.67	9.218	1496	−81.26	0.58
DMP	283.27 to 451.97	9.354	1659	−83.20	0.60

$100\delta P/P = \frac{1}{N}\sum_{i=1}^{N} 100\left(\frac{P_{calc}-P_{exp}}{P_{exp}}\right)$, where N is the total number of experimental values.

TABLE 3
Estimated enthalpies of vaporization of PDA and DMP at $T = 298.15$ K ($\Delta_{\text{vap}}H_{\text{m}}$ ($T = 298.15$)) using equation (4).

Compound	Temperature range/K	T_{m}/K	$\Delta_{\text{vap}}H_{\text{m}}$ (T_{m}) kJ · mol^{-1}	$\Delta_{\text{vap}}H_{\text{m}}$ (298.15) kJ · mol^{-1}
PDA	272.97 to 451.67	376.9	48.8	54.9
DMP	283.27 to 451.97	386.6	54.3	60.9

$\Delta_{\Delta\text{vap}H} = \Delta_{\text{vap}}H_{\text{m}}^{lit}(298.15\text{ K}) - \Delta_{\text{vap}}H_{\text{m}}^{cal}(298.15\text{ K})$.

TABLE 4
Molar fraction of the liquid and vapor phase, x_i; y_i, vapor pressure P, uncertainty $u(P)$ for pressure and activity coefficients γ_1 and γ_2 for the binary system (PDA (1) + water (2)).

x_1[a]	y_1	P/kPa	1000 * $u(P)$/kPa	γ_1	γ_2
		$T = 273.15$ K			
0.0000	0.0000	0.603[b]	18	0.01	1.00
0.1300	0.0007	0.467	14	0.10	0.88
0.2700	0.0107	0.273	8	0.41	0.61
0.3900	0.0489	0.168	5	0.81	0.44
0.4999	0.1183	0.121	4	1.08	0.35
0.6298	0.2094	0.094	3	1.16	0.33
0.7590	0.2834	0.076	2	1.09	0.38
0.8888	0.4069	0.059	2	1.02	0.52
1.0000	1.0000	0.026	1	1.00	0.66
		$T = 283.15$ K			
0.0000	0.0000	1.219[b]	12	0.02	1.00
0.1300	0.0011	0.964	10	0.12	0.89
0.2700	0.0128	0.585	18	0.43	0.65
0.3900	0.0518	0.377	11	0.79	0.49
0.4999	0.1190	0.277	8	1.02	0.40
0.6298	0.2124	0.212	6	1.10	0.37
0.7590	0.3036	0.168	5	1.06	0.40
0.8888	0.4615	0.126	4	1.01	0.50
1.0000	1.0000	0.064	2	1.00	0.57
		$T = 293.15$ K			
0.0000	0.0000	2.329[b]	7	0.03	1.00
0.1300	0.0016	1.877	6	0.15	0.90
0.2700	0.0150	1.178	12	0.46	0.69
0.3900	0.0545	0.792	8	0.78	0.53
0.4999	0.1194	0.594	18	0.98	0.45
0.6298	0.2132	0.451	14	1.05	0.41
0.7590	0.3172	0.351	11	1.03	0.43
0.8888	0.5039	0.255	8	1.00	0.49
1.0000	1.0000	0.144	4	1.00	0.50
		$T = 303.15$ K			
0.0000	0.0000	4.235[b]	13	0.05	1.00
0.1300	0.0022	3.467	10	0.19	0.91
0.2700	0.0174	2.250	7	0.49	0.72
0.3900	0.0573	1.568	5	0.78	0.58
0.4999	0.1200	1.200	12	0.95	0.49
0.6298	0.2129	0.908	9	1.02	0.45
0.7590	0.3255	0.700	7	1.01	0.47
0.8888	0.5340	0.499	15	1.00	0.49
1.0000	1.0000	0.299	9	1.00	0.46
		$T = 313.15$ K			
0.0000	0.0000	7.370[b]	22	0.07	1.00
0.1300	0.0029	6.118	18	0.23	0.93
0.2700	0.0200	4.101	12	0.53	0.76
0.3900	0.0602	2.949	9	0.79	0.62
0.4999	0.1209	2.296	7	0.94	0.54
0.6298	0.2122	1.739	5	1.00	0.50
0.7590	0.3300	1.333	4	1.00	0.51
0.8888	0.5528	0.937	9	0.99	0.51
1.0000	1.0000	0.585	18	1.00	0.45
		$T = 323.15$ K			
0.0000	0.0000	12.330[b]	37	0.11	1.00
0.1300	0.0039	10.360	31	0.28	0.94
0.2700	0.0228	7.166	21	0.57	0.79
0.3900	0.0632	5.294	16	0.80	0.67
0.4999	0.1222	4.188	13	0.94	0.59
0.6298	0.2115	3.189	10	0.99	0.55
0.7590	0.3315	2.438	7	0.99	0.55
0.8888	0.5618	1.701	5	0.99	0.55
1.0000	1.0000	1.081	11	1.00	0.46
		$T = 333.15$ K			
0.0000	0.0000	19.910[b]	60	0.15	1.00
0.1300	0.0050	16.920	51	0.34	0.95
0.2700	0.0258	12.060	36	0.61	0.82
0.3900	0.0665	9.121	27	0.83	0.71
0.4999	0.1238	7.319	22	0.94	0.64
0.6298	0.2111	5.621	17	0.99	0.60
0.7590	0.3308	4.295	13	0.99	0.60
0.8888	0.5626	2.990	9	0.99	0.59
1.0000	1.0000	1.902	6	1.00	0.50