

Supplementary information to “**Complexes of 2,6-dimethylpyridine with water in condensed phases and the dynamical co-operative interactions involving hydrogen bonds**” by W. Marczak, K. Kiełek, B. Czech, H. Flakus and M. Rogalski

The liquidus (T_L) and eutectic (T_E) temperatures, and enthalpies of fusion ($\Delta_f H$) for the system 2,6-dimethylpyridine (1) + water (2) determined calorimetrically

x_1	T_L / K	T_E / K	$\Delta_f H / (\text{kJ mol}^{-1})$
0	273.2		5.99
0.0101	273.7	262.2	5.57
0.0255	273.5	262.5	5.47
0.0501	272.8	262.5	5.18
0.1001	271.3	262.3	4.81
0.2015	263.4		5.04
0.2495	264.0		4.95
0.2983	266.6	261.9	5.22
0.3908	270.9	262.2	6.47
0.3908	270.9	262.1	6.38
0.4513	272.4	261.8	7.05
0.5013	273.0		7.87
0.5470	272.4	257.0	7.65
0.5900	270.8	257.2	8.02
0.5900	271.0	257.5	7.79
0.6347	269.3	257.8	8.02
0.6990	265.2	258.1	8.72
0.7991		257.5	9.48
0.9008	260.9	256.9	10.33
1	266.6		12.74

Coefficients of the polynomials (eq. 2) for density of the system 2,6-dimethylpyridine (1) + water (2) in the temperature limits (273.15 – 293.15 K) and standard deviations of the fit δ

x_1	a_0	a_1	$a_2 \times 10^3$	$a_3 \times 10^5$	δ
0.04987	1005.739 ± 0.001	-0.3460 ± 0.0003	-4.28 ± 0.04	1.3 ± 0.1	0.001
0.10930	1008.899 ± 0.001	-0.6438 ± 0.0002	-2.12 ± 0.01		0.001
0.16637	1008.760 ± 0.002	-0.7864 ± 0.0004	-1.47 ± 0.02		0.002
0.23060	1006.029 ± 0.002	-0.8622 ± 0.0003	-1.18 ± 0.02		0.002
0.28419	1002.418 ± 0.002	-0.8901 ± 0.0004	-1.12 ± 0.02		0.002
0.33272	999.849 ± 0.002	-0.9072 ± 0.0005	-0.89 ± 0.03		0.002
0.37006	995.325 ± 0.001	-0.9110 ± 0.0002	-1.07 ± 0.01		0.001
0.41178	991.609 ± 0.001	-0.9172 ± 0.0002	-0.99 ± 0.01		0.001
0.44399	988.688 ± 0.001	-0.9198 ± 0.0002	-0.95 ± 0.01		0.001
0.47125	986.144 ± 0.001	-0.9215 ± 0.0003	-0.91 ± 0.01		0.001
0.49859	983.577 ± 0.001	-0.9221 ± 0.0003	-0.88 ± 0.01		0.001
0.52137	981.507 ± 0.002	-0.9221 ± 0.0005	-0.85 ± 0.03		0.003
0.56475	977.362 ± 0.000	-0.9197 ± 0.0003	-0.71 ± 0.04		0.001
0.66571	967.603 ± 0.000	-0.9054 ± 0.0001	-0.77 ± 0.00		0.000
0.78828	956.307 ± 0.001	-0.8906 ± 0.0001	-0.64 ± 0.01		0.001
0.90276	947.095 ± 0.002	-0.8854 ± 0.0004	-0.49 ± 0.02		0.002
1	940.330 ± 0.001	-0.8851 ± 0.0002	-0.30 ± 0.01		0.001