Electronic Supplementary Material (ESI) for RSC Advances

Supplementary information to "**Water-induced aggregation and hydrophobic hydration in aqueous solutions of N-methylpiperidine**" by W. Marczak, M. Łężniak, M. Zorębski, P. Lodowski, A. Przybyła, D. Truszkowska, and L. Almásy

Mole fractions and temperatures of the cloud points for N-methylpiperidine (1) + water (2)

x_1	T / K
0.0147	327.56
0.0181	322.48
0.0199	321.05
0.0225	320.22
0.0248	320.01
0.0267	319.65
0.0300	317.65
0.0595	316.65
0.0795	316.65
0.0991	316.65
0.1301	317.25
0.1501	318.65
0.1797	320.49
0.1992	321.94
0.2191	323.70
0.2507	325.99
0.2804	326.44
0.3002	329.35
0.3311	330.34
0.3509	333.75
0.3802	336.35
0.4014	339.75
0.4396	340.88
0.4814	342.56

Reduced ultrasonic absorption, $\alpha\,\nu^{-2} \times 10^{15}$ / (s^2 m^{-1}), in N-methylpiperidine (1) + water (2) at T = 293.15 K

ν / MHz	x_1						
	0	0.0051	0.030	0.070	0.100	0.300	1
10.00	27.71	120.4	1668	1276	972	487	239
12.51	26.62	115.5	1514	1211	917	429	239
15.01	26.60	108.4	1375	1136	885	400	233
18.01	25.79	103.4	1234	1072	832	368	229
22.12	25.28	93.8	1071	988	777	343	220
26.58	24.56	86.8	935	919	737	325	210
30.00	28.34	86.4	878	860	695	321	200
39.00	26.93	69.9	698	762	627	296	189
47.00	26.64	60.6	574	684	575	283	173
56.00	25.91	53.3	477	608	526	271	157
69.00	25.78	46.0	376	525	471	255	139
79.00	25.91	41.9	324	475	438	247	128
100.00	26.14	37.2	253	407	390	235	117

ν / MHz	x_1	
	0.020	0.040
12.50	496	1592
15.05	438	1463
18.00	435	1334
22.12	384	1180
26.59	365	1062
30.00	355	995
39.00	294	833
47.00	249	724
56.00	210	614
69.00	168	498
79.00	147	433
100.00	114	344

ν / MHz	x_1
	0.050
12.50	1501
15.01	1391
18.00	1263
22.12	1175
26.59	1077
30.00	987
39.00	849
47.00	737
56.00	640
69.00	530
79.00	467
100.00	383

ν / MHz	x_1		
	0.500	0.700	0.900
10.00	431	346	254
12.51	383	327	254
15.01	341	303	248
18.01	298	278	240
22.12	258	244	228
26.58	228	219	212
30.00	209	202	204
36.06	190	171	183
39.55	180	158	
45.03	170	150	162
52.50	161	136	146
60.10	151	124	134
69.94	141	113	124
79.14	135	108	113

Densities of the system N-methylpiperidine (1) + water (2)

x_1	t / °C	ρ/ (kg m^{-3})	x_1	t / °C	ρ/ (kg m^{-3})	x_1	t / °C	ρ/ (kg m^{-3})
0.00034	15.005	998.924	0.07007	15.005	967.542	0.39772	15.004	882.524
	19.998	998.026		19.995	964.078		19.998	877.931
	24.996	996.864		24.995	960.542		24.995	873.284
	29.996	995.466		29.999	956.915		29.996	868.596
	34.996	993.852		34.996	953.161		34.994	863.859
	39.996	992.018		39.995	949.217		39.997	859.072
0.00067	15.005	998.743	0.07999	15.002	963.208	0.49990	15.006	866.879
	19.998	997.843		19.998	959.605		19.998	862.309
	24.997	996.677		24.996	955.930		24.995	857.696
	29.996	995.274		29.994	952.163		29.996	853.046
	34.995	993.656		34.994	948.275		34.995	848.353
	39.999	991.785		39.997	944.199		39.998	843.623
0.00364	15.006	997.244	0.09000	15.005	958.986	0.59999	15.002	854.228
	19.996	996.297		19.998	955.264		19.998	849.708
	24.994	995.088		24.995	951.466		24.995	845.146
	29.999	993.639		29.996	947.581		29.994	840.551
	34.996	991.970		34.994	943.570		34.994	835.924
	39.995	990.103		39.998	939.491		40.000	831.256
0.01002	15.005	994.688	0.09996	15.002	955.153	0.69954	15.005	843.321
	19.995	993.566		19.998	951.334		19.996	838.839
	24.995	992.180		24.995	947.434		24.994	834.319
	29.995	990.559		29.995	943.446		29.995	829.771
	34.999	988.717		34.994	939.340		34.996	825.187
	39.996	986.673					39.995	820.573
0.02001	15.004	991.484	0.15027	15.005	937.534	0.79981	15.005	834.283
	19.994	989.799		19.995	933.357		19.994	829.821
	24.995	987.844		24.994	929.101		24.998	825.324
	29.995	985.656		29.995	924.764		29.996	820.802
	34.999	983.269		34.999	920.320		34.996	816.253
	39.995	980.695		39.996	915.744		39.995	811.673
0.03066	15.004	986.974	0.17554	15.001	930.051	0.89918	15.006	826.487
	19.993	984.544		19.998	925.764		19.998	822.037
	24.999	981.967		24.994	921.397		24.997	817.556
	29.996	979.252		29.995	916.951		29.995	813.057
	34.996	976.395		34.998	912.412		34.995	808.536
	39.995	973.377		39.996	907.753		39.995	803.991
0.04001	15.005	982.637	0.20002	15.005	923.044	1[a]	15.002	819.673
	19.996	979.857		19.996	918.739		19.998	815.251
	24.995	976.975		24.994	914.301		24.994	810.808
	29.995	973.988		29.996	909.778		29.996	806.353
	34.998	970.870		34.994	905.170		34.996	801.884
	39.994	967.579		39.995	900.461		39.998	797.400
0.05001	15.005	977.205	0.20706	15.005	921.495	1	15.005	819.748
	19.995	974.124		19.999	917.107		19.998	815.326
	24.994	970.962		24.994	912.641		24.995	810.886
	29.995	967.710		29.995	908.100		29.995	806.431
	34.995	964.362		34.994	903.476		34.994	801.965
	39.995	961.059		39.996	898.751		39.995	797.479
0.06008	15.004	972.117	0.29993	15.002	900.756			
	19.995	968.821		19.998	896.209			
	24.995	965.451		24.995	891.596			
	29.995	961.986		29.996	886.927			
	34.998	958.400		34.994	882.197			
	39.996	954.750		39.994	877.397			

[a]chemical used in the thermodynamic experiments

Coefficients a_i for the molar volume polynomials of N-methylpiperidine (1) + water (2):

$$\ln V/(\mathrm{m^3\ mol^{-1}}) = \sum_{i=0}^{2} a_i (T/\mathrm{K} - 298.15)^i \qquad \text{(Eq. 6)}$$

in the temperature range $T = (288.15 - 315.15)$ K, with the average absolute deviations of the back-calculated densities δ

x_1	a_0	$a_1 \times 10^4$	$a_2 \times 10^6$	δ / (kg m^{-3})
0.00034	2.89589	2.54728	4.68731	0.008
0.00067	2.89755	2.55886	4.81069	0.005
0.00364	2.91243	2.65034	4.66535	0.010
0.01002	2.94322	3.01026	4.68173	0.009
0.02001	2.98979	4.16058	4.55624	0.014
0.03066	3.03879	5.39265	3.10422	0.004
0.04001	3.08023	6.03160	2.73843	0.015
0.05001	3.12388	6.60224	1.56354	0.017
0.06008	3.16593	7.10168	2.19007	0.006
0.07007	3.20581	7.49786	2.71609	0.023
0.07999	3.24401	7.82335	2.70412	0.020
0.09000	3.28132	8.10113	2.28835	0.006
0.09996	3.31700	8.34611	2.32569	0.005
0.15027	3.48175	9.27312	2.52528	0.013
0.17554	3.55574	9.58023	2.42999	0.009
0.20002	3.62325	9.78579	2.57248	0.004
0.20706	3.64159	9.88190	2.27983	0.005
0.29993	3.86089	10.41531	1.92782	0.002
0.39772	4.05337	10.69395	1.63448	0.001
0.49990	4.22402	10.80647	1.47901	0.001
0.59999	4.36861	10.83567	1.39388	0.001
0.69954	4.49582	10.87391	1.34518	0.002
0.79981	4.60994	10.92948	1.27091	0.001
0.89918	4.71221	10.98641	1.13189	0.001
1[a]	4.80660	10.97474	0.93698	0.001
1	4.80657	10.96702	0.93349	0.002

[a]chemical used in the thermodynamic experiments

Speed of ultrasound in the system N-methylpiperidine (1) + water (2)

x_1	t / °C	u / (m s^{-1})	x_1	t / °C	u / (m s^{-1})	x_1	t / °C	u / (m s^{-1})
0.00034	19.41	1482.51	0.06008	18.52	1541.06	0.39772	19.50	1380.16
	24.39	1496.86		23.34	1531.43		24.35	1359.59
	28.62	1507.62		27.54	1522.11		28.42	1342.37
	33.53	1518.36		32.46	1509.73		33.32	1321.70
	38.50	1527.58		37.43	1495.22		38.36	1300.56
0.00067	19.43	1484.47	0.07007	19.40	1532.86	0.49990	19.35	1349.16
	24.39	1498.60		24.36	1521.36		24.30	1327.90
	28.64	1509.23		28.64	1510.46		28.57	1309.74
	33.54	1519.85		33.60	1496.27		33.58	1288.58
	38.52	1528.87		38.58	1479.67		38.64	1267.34
0.00364	19.44	1501.73	0.07999	19.39	1526.71	0.59999	19.46	1322.99
	24.34	1514.12		24.37	1513.99		24.38	1301.86
	28.60	1523.49		28.67	1501.98		28.59	1283.88
	33.51	1532.73		33.64	1486.52		33.50	1263.07
	38.51	1540.46		38.64	1468.66		38.46	1242.27
0.01002	19.46	1535.74	0.09000	19.47	1520.09	0.69954	19.44	1302.00
	24.37	1544.63		24.27	1506.67		24.33	1280.84
	28.56	1550.89		28.51	1494.03		28.58	1262.66
	33.50	1556.81		33.52	1477.72		33.48	1241.84
	38.46	1561.23		38.47	1459.20		38.46	1220.86
0.02001	19.40	1567.30	0.09996	19.39	1514.65	0.79981	19.45	1284.75
	24.37	1566.60		24.38	1499.98		24.37	1263.27
	28.63	1565.28		28.66	1486.45		28.60	1245.02
	33.59	1562.98		33.62	1469.42		33.50	1224.02
	38.66	1560.04		38.61	1450.47		38.47	1202.96
0.03066	18.47	1562.79	0.15027	19.53	1486.37	0.89918	19.44	1270.87
	23.38	1558.06		24.39	1469.18		24.38	1249.10
	27.05	1554.33		28.60	1453.62		28.60	1230.62
	32.48	1547.92		33.45	1434.89		33.47	1209.51
	37.44	1541.31		38.42	1414.55		38.44	1188.24
0.04001	19.40	1554.14	0.20002	19.47	1460.82	1	19.45	1259.66
	24.39	1547.49		24.37	1442.16		24.37	1237.58
	28.66	1541.30		28.59	1425.65		28.62	1218.82
	33.59	1532.91		33.51	1405.87		33.56	1197.30
	38.57	1522.52		38.47	1385.29		38.52	1175.99
0.05001	19.41	1546.48	0.29993	19.38	1417.08			
	24.38	1538.03		24.36	1396.71			
	28.67	1529.92		28.66	1379.06			
	33.63	1518.92		33.64	1358.40			
	38.62	1506.05		38.65	1337.48			

Coefficients of the speed of sound polynomials for N-methylpiperidine (1) + water (2):

$$u/(\mathrm{m\,s^{-1}}) = \sum_{i=0}^{n} b_i (T/\mathrm{K} - 298.15)^i \qquad \text{(Eq. 7)}$$

and standard deviations of the fit δ

x_1	b_0	b_1	$b_2 \times 10^3$	$b_3 \times 10^4$	δ
0.00034	1498.477 ± 0.032	2.6497 ± 0.0059	-3.674 ± 0.060		0.05
0.00067	1500.193 ± 0.013	2.6162 ± 0.0025	-3.663 ± 0.025		0.02
0.00364	1515.640 ± 0.014	2.3055 ± 0.0027	-3.471 ± 0.027		0.02
0.01002	1545.613 ± 0.025	1.5999 ± 0.0047	-3.276 ± 0.048		0.04
0.02001	1566.391 ± 0.041	-0.2549 ± 0.0077	-1.553 ± 0.077		0.07
0.03066	1556.450 ± 0.055	-1.0363 ± 0.0118	-1.172 ± 0.173	-0.23 ± 0.18	0.07
0.04001	1546.650 ± 0.021	-1.3961 ± 0.0034	-1.566 ± 0.076	-0.92 ± 0.06	0.02
0.05001	1536.938 ± 0.055	-1.8291 ± 0.0088	-2.495 ± 0.198	-0.53 ± 0.15	0.06
0.06008	1527.866 ± 0.010	-2.1979 ± 0.0020	-2.602 ± 0.032	-0.67 ± 0.03	0.01
0.07007	1519.797 ± 0.015	-2.4543 ± 0.0025	-2.614 ± 0.055	-0.79 ± 0.04	0.02
0.07999	1512.288 ± 0.017	-2.6977 ± 0.0028	-2.676 ± 0.061	-0.73 ± 0.05	0.02
0.09000	1504.543 ± 0.045	-2.8984 ± 0.0074	-2.111 ± 0.166	-1.01 ± 0.13	0.05
0.09996	1498.069 ± 0.006	-3.0768 ± 0.0010	-2.456 ± 0.023	-0.46 ± 0.02	0.01
0.15027	1466.963 ± 0.016	-3.6349 ± 0.0027	-1.732 ± 0.061	-0.21 ± 0.05	0.02
0.20002	1439.736 ± 0.014	-3.8769 ± 0.0026	-1.227 ± 0.026		0.02
0.29993	1394.095 ± 0.015	-4.1030 ± 0.0027	-0.324 ± 0.027		0.02
0.39772	1356.824 ± 0.018	-4.2335 ± 0.0035	0.167 ± 0.036		0.03
0.49990	1324.937 ± 0.007	-4.2653 ± 0.0013	0.323 ± 0.013		0.01
0.59999	1299.185 ± 0.009	-4.2757 ± 0.0017	0.359 ± 0.018		0.02
0.69954	1277.970 ± 0.016	-4.2974 ± 0.0029	0.400 ± 0.029		0.03
0.79981	1260.553 ± 0.013	-4.3342 ± 0.0024	0.434 ± 0.024		0.02
0.89918	1246.365 ± 0.013	-4.3858 ± 0.0025	0.452 ± 0.025		0.02
1	1234.799 ± 0.008	-4.4396 ± 0.0015	0.664 ± 0.016		0.01

Coefficients of the empirical polynomial:

$$\frac{Z^{\mathrm{E}}}{x_1 x_2} = \sum_{i=0}^{5}\sum_{j=0}^{3} a_{ij} c^i \vartheta^j , \qquad \text{(Eq. 15)}$$

for the excess molar volumes $Z = V \times 10^6/(\mathrm{m^3\ mol^{-1}})$ at $T = (288.15 - 313.15)$ K and for the excess molar isentropic compressions $Z = K_S \times 10^{15}/(\mathrm{m^3\ mol^{-1}\ Pa^{-1}})$ at $T = (291.15 - 311.15)$ K. $c = x_1/(x_1 + x_2/15)$, $\vartheta = T/\mathrm{K} - 298.15$, r is the correlation coefficient

		V^{E}; $r = 0.9980$		K_S^{E}; $r = 0.9987$	
i	j	$a_{ij} \times 10^n$	n	$a_{ij} \times 10^n$	n
0	0	-128.75 ± 0.48	1	-128.75 ± 0.46	0
0	1	-1.21 ± 0.11	1	2.73 ± 0.61	1
0	2	0		-1.69 ± 0.81	2
0	3	4.28 ± 0.72	4	0.60 ± 0.54	3
1	0	-8.55 ± 0.43	0	0	
1	1	10.14 ± 0.89	1	0	
1	2	0		0	
1	3	-0.58 ± 0.11	2	0	
2	0	0		6.17 ± 0.10	-2
2	1	-1.31 ± 0.16	0	0.32 ± 0.12	-1
2	2	0		1.26 ± 0.82	2
2	3	2.88 ± 0.71	2	0	
3	0	15.21 ± 0.48	-1	-10.90 ± 0.24	-2
3	1	0		-1.00 ± 0.29	-1
3	2	0		0	
3	3	-0.66 ± 0.18	1	0	
4	0	-27.83 ± 0.89	-1	5.68 ± 0.15	-2
4	1	4.31 ± 0.85	1	0.63 ± 0.18	-1
4	2	0		0	
4	3	0.70 ± 0.20	1	0	
5	0	14.23 ± 0.45	-1	0	
5	1	0		0	
5	2	0		0	
5	3	-2.73 ± 0.81	2	0	