

Supplementary Data

Experimental and theoretical studies of transport and optical properties of binary mixtures of acetonitrile with some alkyl methacrylates at temperatures from 298.15 to 318.15 K

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Table S1 — Deviations in viscosity, $\Delta\eta$ as function of mole fraction, x_1 of ACN for ACN + MMA/EMA/ *n*-BMA mixtures at the temperatures, $T = (298.15 - 318.15)$ K and atmospheric pressure

x_1	$10^4 \times \Delta\eta (\text{N s m}^{-2})$ at T/K				
	298.15	303.15	308.15	313.15	318.15
<u>ACN + MMA</u>					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0688	0.0598	0.0640	0.0676	0.0725	0.0761
0.1376	0.1116	0.1170	0.1221	0.1279	0.1332
0.1957	0.1443	0.1513	0.1588	0.1647	0.1714
0.2716	0.1765	0.1840	0.1909	0.1989	0.2078
0.3344	0.1923	0.2014	0.2089	0.2174	0.2264
0.4135	0.2014	0.2103	0.2187	0.2279	0.2368
0.4916	0.1993	0.2083	0.2177	0.2266	0.2357
0.5649	0.1889	0.1960	0.2042	0.2145	0.2229
0.6386	0.1693	0.1774	0.1844	0.1941	0.2018
0.7084	0.1453	0.1523	0.1587	0.1672	0.1745
0.7927	0.1096	0.1153	0.1207	0.1282	0.1342
0.8550	0.0794	0.0847	0.0888	0.0929	0.0980
0.9073	0.0515	0.0548	0.0582	0.0611	0.0640
0.9497	0.0282	0.0308	0.0321	0.0341	0.0362
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<u>ACN + EMA</u>					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0556	0.0370	0.0400	0.0430	0.0465	0.0491
0.1112	0.0700	0.0750	0.0790	0.0841	0.0891
0.1631	0.0961	0.1017	0.1080	0.1136	0.1200
0.2147	0.1154	0.1236	0.1303	0.1376	0.1454
0.2795	0.1355	0.1448	0.1522	0.1605	0.1689
0.3446	0.1496	0.1577	0.1666	0.1758	0.1849
0.4132	0.1559	0.1654	0.1747	0.1838	0.1937
0.4819	0.1566	0.1654	0.1749	0.1850	0.1947
0.5597	0.1501	0.1583	0.1678	0.1772	0.1869
0.6375	0.1356	0.1442	0.1527	0.1615	0.1702
0.7251	0.1120	0.1198	0.1268	0.1342	0.1428
0.8113	0.0823	0.0879	0.0938	0.1002	0.1061
0.9014	0.0451	0.0487	0.0522	0.0566	0.0599
0.9542	0.0209	0.0227	0.0252	0.0269	0.0293
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<u>ACN + <i>n</i>-BMA</u>					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0681	0.0293	0.0318	0.0341	0.0358	0.0378
0.1359	0.0541	0.0582	0.0618	0.0655	0.0695
0.1976	0.0735	0.0786	0.0832	0.0879	0.0925
0.2728	0.0905	0.0963	0.1020	0.1079	0.1127
0.3442	0.1013	0.1078	0.1143	0.1209	0.1268
0.4143	0.1073	0.1142	0.1209	0.1277	0.1341
0.4658	0.1085	0.1159	0.1223	0.1295	0.1360
0.5243	0.1079	0.1149	0.1209	0.1281	0.1351
0.5649	0.1054	0.1126	0.1182	0.1256	0.1314
0.6390	0.0975	0.1040	0.1102	0.1163	0.1216
0.7112	0.0856	0.0914	0.0960	0.1014	0.1066
0.7836	0.0698	0.0738	0.0786	0.0824	0.0865
0.8558	0.0499	0.0532	0.0563	0.0595	0.0626
0.9280	0.0270	0.0286	0.0301	0.0317	0.0337
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table S2 — Deviations in refractive index, Δn_D as function of mole fraction, x_1 of ACN for ACN + MMA/EMA/*n*-BMA mixtures at the temperatures, $T = (298.15 - 318.15)$ K and atmospheric pressure

x_1	$10^2 \times \Delta n_D$ at T/K				
	298.15	303.15	308.15	313.15	318.15
<u>ACN + MMA</u>					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0688	0.1042	0.1125	0.1222	0.1322	0.1335
0.1376	0.2069	0.2134	0.2233	0.2333	0.2554
0.1957	0.2850	0.2998	0.3095	0.3301	0.3429
0.2716	0.3810	0.3942	0.4134	0.4340	0.4577
0.3344	0.4429	0.4640	0.4835	0.5141	0.5386
0.4135	0.5196	0.5378	0.5659	0.5973	0.6229
0.4916	0.5654	0.5904	0.6186	0.6493	0.6869
0.5649	0.5904	0.6127	0.6396	0.6709	0.7098
0.6386	0.5821	0.6108	0.6375	0.6689	0.6993
0.7084	0.5451	0.5697	0.5957	0.6271	0.6591
0.7927	0.4574	0.4759	0.5008	0.5321	0.5557
0.8550	0.3555	0.3694	0.3934	0.4141	0.4294
0.9073	0.2406	0.2602	0.2726	0.2833	0.3004
0.9497	0.1381	0.1439	0.1556	0.1655	0.1742
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<u>ACN + EMA</u>					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0556	0.0752	0.0852	0.0950	0.0952	0.1062
0.1112	0.1428	0.1520	0.1615	0.1727	0.1855
0.1631	0.2003	0.2181	0.2380	0.2495	0.2633
0.2147	0.2488	0.2764	0.2961	0.3179	0.3335
0.2795	0.3085	0.3350	0.3651	0.3872	0.4143
0.3446	0.3651	0.3912	0.4201	0.4533	0.4820
0.4132	0.4090	0.4343	0.4635	0.4972	0.5278
0.4819	0.4321	0.4659	0.4945	0.5295	0.5622
0.5597	0.4507	0.4817	0.5104	0.5460	0.5722
0.6375	0.4383	0.4677	0.4956	0.5321	0.5513
0.7251	0.4011	0.4275	0.4444	0.4719	0.4951
0.8113	0.3290	0.3518	0.3668	0.3855	0.4034
0.9014	0.2080	0.2257	0.2392	0.2486	0.2618
0.9542	0.1041	0.1079	0.1204	0.1301	0.1367
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<u>ACN + <i>n</i>-BMA</u>					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0681	0.0457	0.0570	0.0688	0.0807	0.0731
0.1359	0.1101	0.1228	0.1363	0.1505	0.1455
0.1976	0.1547	0.1786	0.1940	0.2103	0.2181
0.2728	0.2155	0.2312	0.2592	0.2782	0.2996
0.3442	0.2568	0.2744	0.3050	0.3271	0.3522
0.4143	0.2925	0.3121	0.3455	0.3709	0.4001
0.4658	0.3165	0.3377	0.3635	0.3915	0.4242
0.5243	0.3257	0.3489	0.3775	0.4089	0.4358
0.5649	0.3315	0.3562	0.3871	0.4109	0.4410
0.6390	0.3323	0.3501	0.3754	0.4044	0.4310
0.7112	0.3125	0.3336	0.3538	0.3786	0.4025
0.7836	0.2690	0.2840	0.3000	0.3215	0.3441
0.8558	0.2132	0.2225	0.2353	0.2547	0.2675
0.9280	0.1256	0.1300	0.1406	0.1495	0.1645
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table S3 — Deviations in molar refraction, ΔR_M as function of mole fraction, x_1 of ACN for ACN + MMA/EMA/*n*-BMA mixtures at the temperatures, $T = (298.15 - 318.15)$ K and atmospheric pressure

x_1	$10^6 \times \Delta R_M$ ($\text{m}^3 \text{mol}^{-1}$) at T/K				
	298.15	303.15	308.15	313.15	318.15
<u>ACN + MMA</u>					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0688	0.0457	0.0499	0.0550	0.0605	0.0609
0.1376	0.0906	0.0936	0.0982	0.1035	0.1151
0.1957	0.1234	0.1307	0.1352	0.1454	0.1520
0.2716	0.1625	0.1685	0.1776	0.1878	0.1997
0.3344	0.1858	0.1954	0.2042	0.2188	0.2310
0.4135	0.2128	0.2208	0.2336	0.2480	0.2604
0.4916	0.2251	0.2357	0.2479	0.2617	0.2787
0.5649	0.2285	0.2373	0.2487	0.2618	0.2786
0.6386	0.2184	0.2291	0.2397	0.2525	0.2652
0.7084	0.1981	0.2068	0.2166	0.2287	0.2414
0.7927	0.1594	0.1658	0.1746	0.1857	0.1948
0.8550	0.1199	0.1245	0.1325	0.1396	0.1453
0.9073	0.0790	0.0851	0.0892	0.0928	0.0986
0.9497	0.0444	0.0460	0.0496	0.0529	0.0557
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<u>ACN + EMA</u>					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0556	0.0410	0.0468	0.0531	0.0531	0.0470
0.1112	0.0758	0.0808	0.0865	0.0931	0.1005
0.1631	0.1039	0.1144	0.1256	0.1321	0.1403
0.2147	0.1261	0.1416	0.1528	0.1649	0.1737
0.2795	0.1520	0.1663	0.1825	0.1947	0.2098
0.3446	0.1746	0.1876	0.2034	0.2211	0.2368
0.4132	0.1887	0.2007	0.2157	0.2332	0.2494
0.4819	0.1914	0.2071	0.2210	0.2381	0.2549
0.5597	0.1903	0.2045	0.2176	0.2340	0.2466
0.6375	0.1761	0.1883	0.2003	0.2164	0.2251
0.7251	0.1515	0.1617	0.1686	0.1797	0.1895
0.8113	0.1164	0.1247	0.1304	0.1373	0.1443
0.9014	0.0683	0.0741	0.0787	0.0821	0.0867
0.9542	0.0327	0.0339	0.0376	0.0408	0.0431
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<u>ACN + <i>n</i>-BMA</u>					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0681	0.0332	0.0422	0.0517	0.0614	0.0553
0.1359	0.0788	0.0884	0.0992	0.1102	0.1064
0.1976	0.1072	0.1246	0.1362	0.1486	0.1549
0.2728	0.1434	0.1542	0.1740	0.1878	0.2035
0.3442	0.1635	0.1749	0.1952	0.2106	0.2280
0.4143	0.1779	0.1898	0.2110	0.2278	0.2470
0.4658	0.1855	0.1981	0.2138	0.2315	0.2522
0.5243	0.1831	0.1962	0.2125	0.2312	0.2477
0.5649	0.1806	0.1940	0.2111	0.2251	0.2426
0.6390	0.1705	0.1797	0.1927	0.2081	0.2225
0.7112	0.1508	0.1608	0.1705	0.1826	0.1950
0.7836	0.1217	0.1284	0.1355	0.1451	0.1556
0.8558	0.0897	0.0937	0.0989	0.1068	0.1124
0.9280	0.0490	0.0507	0.0546	0.0579	0.0635
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table S4 — The values of activation energy, E_a and Arrhenius factor, A_s of activation of viscous flow along with the linear regression coefficient, r^2 as a function of mole fraction, x_1 of ACN for ACN + MMA/EMA/ *n*-BMA binary mixtures

x_1	E_a (kJ mol ⁻¹)	A_s (J mol ⁻¹)	r^2	x_1	E_a (kJ mol ⁻¹)	A_s (J mol ⁻¹)	r^2
<u>ACN + MMA</u>							
0.0000	8.839	15.783	0.993	0.5649	7.207	24.957	0.996
0.0688	8.497	17.835	0.993	0.6386	7.089	25.163	0.997
0.1376	8.260	19.282	0.993	0.7084	6.997	25.100	0.998
0.1957	8.064	20.517	0.993	0.7927	6.893	24.852	0.999
0.2716	7.847	21.856	0.994	0.8550	6.855	24.219	0.999
0.3344	7.681	22.834	0.994	0.9073	6.828	23.600	1.000
0.4135	7.498	23.814	0.995	0.9497	6.808	23.066	1.000
0.4916	7.331	24.608	0.996	1.0000	6.813	22.164	1.000
<u>ACN + EMA</u>							
0.0000	13.266	3.022	0.998	0.4819	10.222	8.290	0.998
0.0556	12.853	3.500	0.998	0.5597	9.761	9.532	0.998
0.1112	12.485	3.974	0.998	0.6375	9.289	10.963	0.998
0.1631	12.154	4.449	0.998	0.7251	8.736	12.886	0.999
0.2147	11.821	4.978	0.998	0.8113	8.168	15.164	0.999
0.2795	11.431	5.658	0.998	0.9014	7.536	18.139	1.000
0.3446	11.042	6.413	0.998	0.9542	7.145	20.244	1.000
0.4132	10.632	7.301	0.998	1.0000	6.813	22.164	1.000
<u>ACN + <i>n</i>-BMA</u>							
0.0000	11.019	10.222	0.996	0.5243	9.278	14.362	0.997
0.0681	10.799	10.748	0.996	0.5649	9.127	14.722	0.997
0.1359	10.580	11.276	0.996	0.6390	8.829	15.475	0.998
0.1976	10.388	11.727	0.996	0.7112	8.519	16.284	0.998
0.2728	10.149	12.281	0.997	0.7836	8.173	17.258	0.999
0.3442	9.910	12.854	0.997	0.8558	7.777	18.520	0.999
0.4143	9.674	13.409	0.997	0.9280	7.335	20.053	1.000
0.4658	9.491	13.850	0.997	1.0000	6.813	22.164	1.000

Table S5 — Partial molar activation energies $E_{a,1}$ and $E_{a,2}$ of the components (ACN and alkyl acrylates) as function of mole fraction, x_1
 ACN of for ACN + alkyl methacrylate mixtures in the temperature range, $T = (298.15 - 318.15)$ K

x_1	$E_{a,1}$ (kJ mol ⁻¹)	$E_{a,2}$ (kJ mol ⁻¹)	x_1	$E_{a,1}$ (kJ mol ⁻¹)	$E_{a,2}$ (kJ mol ⁻¹)	x_1	$E_{a,1}$ (kJ mol ⁻¹)	$E_{a,2}$ (kJ mol ⁻¹)
<u>ACN + MMA</u>				<u>ACN + EMA</u>			<u>ACN + n-BMA</u>	
0.0000	4.9027	8.8386	0.0000	7.3124	13.2658	0.0000	8.7942	11.0194
0.0688	5.0836	8.7491	0.0556	7.1941	13.1858	0.0681	8.4985	10.9672
0.1376	5.3323	8.7273	0.1112	7.1257	13.1557	0.1359	8.2377	10.9488
0.1957	5.5176	8.6842	0.1631	7.0779	13.1435	0.1976	8.0350	10.9668
0.2716	5.7574	8.6257	0.2147	7.0296	13.1308	0.2728	7.8213	11.0221
0.3344	5.9367	8.5581	0.2795	7.0029	13.1487	0.3442	7.6438	11.0999
0.4135	6.1433	8.4538	0.3446	6.9845	13.1751	0.4143	7.5031	11.2099
0.4916	6.3122	8.3157	0.4132	6.9716	13.2094	0.4658	7.4127	11.3037
0.5649	6.4607	8.1760	0.4819	6.9658	13.2508	0.5243	7.3280	11.4281
0.6386	6.5742	7.9997	0.5597	6.9697	13.3084	0.5649	7.2800	11.5253
0.7084	6.6616	7.8128	0.6375	6.9721	13.3642	0.6390	7.2012	11.7116
0.7927	6.7229	7.5426	0.7251	6.9617	13.4142	0.7112	7.1414	11.9099
0.8550	6.7715	7.3464	0.8113	6.9389	13.4507	0.7836	7.0853	12.1127
0.9073	6.7940	7.1633	0.9014	6.8877	13.4615	0.8558	7.0147	12.3004
0.9497	6.7981	7.0007	0.9542	6.8420	13.4521	0.9280	6.9354	12.4792
1.0000	6.8127	6.8175	1.0000	6.8127	13.4543	1.0000	6.8127	12.6140

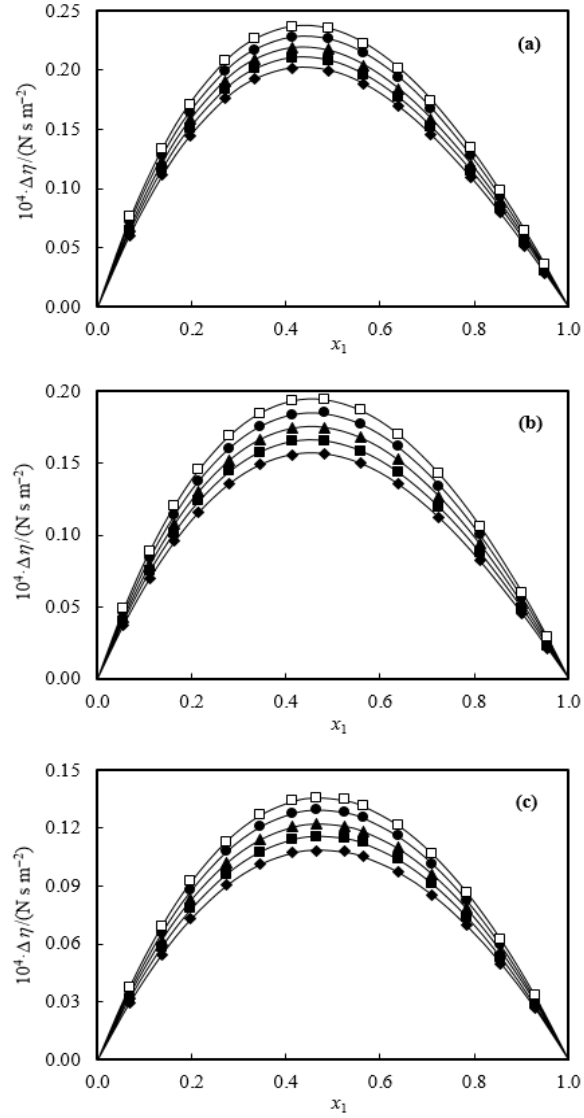


Fig. S1 — Plots of deviations in viscosity, $\Delta\eta$ vs. mole fraction, x_1 of ACN for (a) ACN + MMA, (b) ACN + EMA and (c) ACN + BMA binary mixtures at temperatures, $T/K = 298.15$, ◆; At $T/K = 303.15$, ■; $T/K = 308.15$, ▲; $T/K = 313.15$, ×; $T/K = 318.15$, □. The points represent experimental values and lines represent values calculated from equation (7).

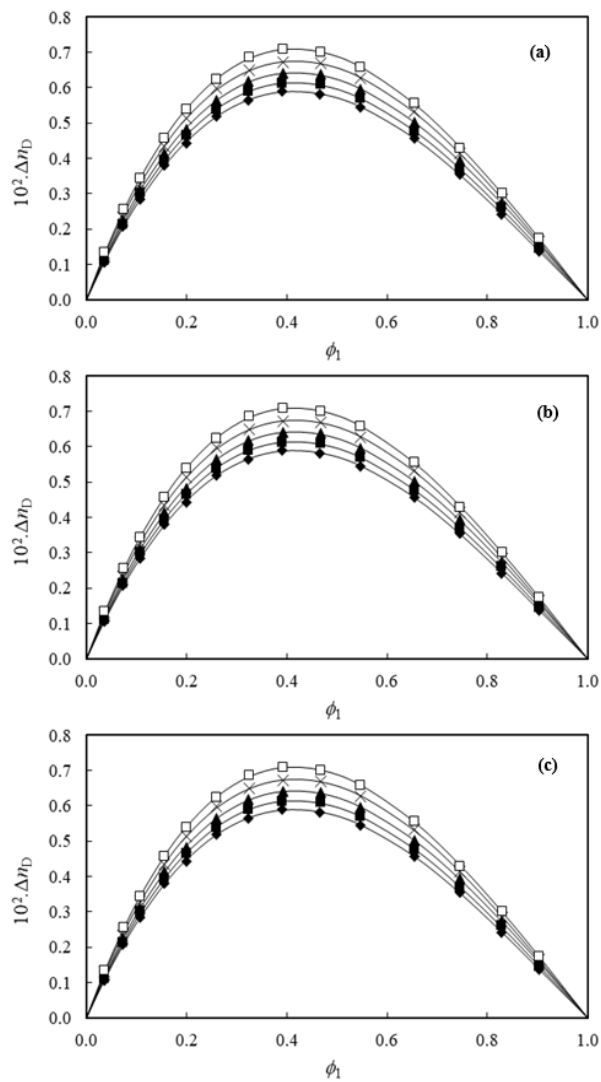


Fig. S2 — Plots of deviation in refractive index, Δn_D vs. volume fraction, ϕ_1 of ACN for (a) ACN + MMA, (b) ACN + EMA and (c) ACN + BMA binary mixtures at temperatures, $T/K = 298.15$, \blacklozenge ; At $T/K = 303.15$, \blacksquare ; $T/K = 308.15$, \blacktriangle ; $T/K = 313.15$, \times ; $T/K = 318.15$, \square . The points represent experimental values and lines represent values calculated from equation (7).

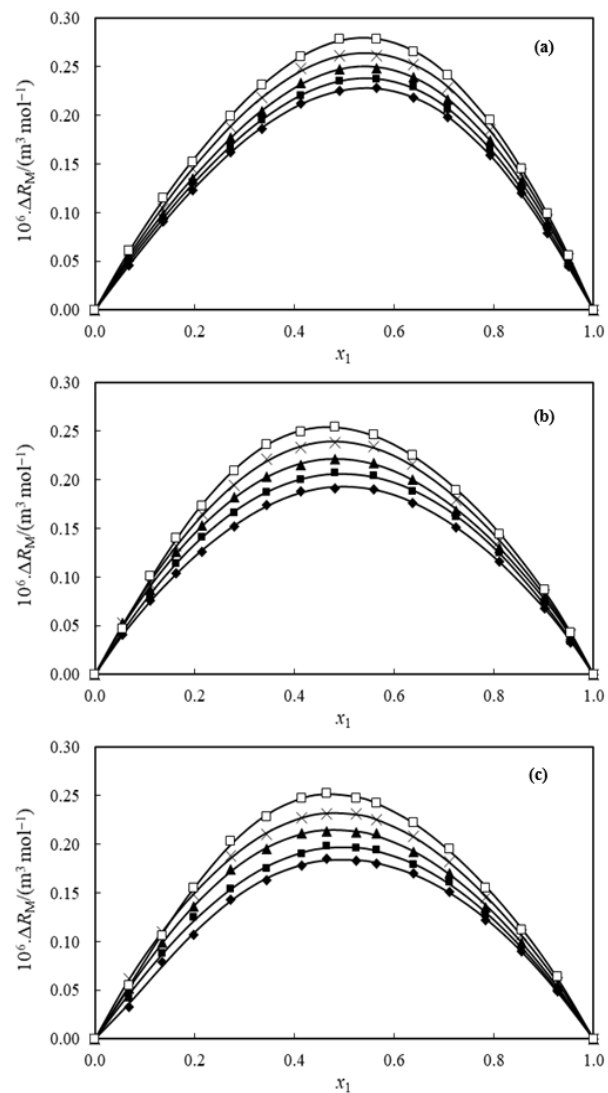


Fig. S3 — Plots of deviations in molar refractions, ΔR_M vs. mole fraction, x_1 of ACN for (a) ACN + MMA, (b) ACN + EMA and (c) ACN + BMA binary mixtures at temperatures, $T/K = 298.15$, \blacklozenge ; At $T/K = 303.15$, \blacksquare ; $T/K = 308.15$, \blacktriangle ; $T/K = 313.15$, \times ; $T/K = 318.15$, \square . The points represent experimental values and lines represent values calculated from equation (7).