Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

Dipole moments of isomeric alkoxyalcohols in cyclohexane. Comparison of Hedestrand and Fröhlich procedures with a new formula

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TABLE S1 Densities ρ / g cm^{-3} of solutions of 1-propoxypropan-2-ol (1-pp-2-ol), 2-butoxyethanol (nC$_4$E$_1$), 2-isobutoxyethanol (iC$_4$E$_1$) and 2-*tert*-butoxyethanol (tC$_4$E$_1$) at different mole fractions x_2 in cyclohexane at T = 298.15 K

x_2	ρ / g cm^{-3}	x_2	ρ / g cm^{-3}
1-pp-2-ol		nC$_4$E$_1$	
0.00000	0.773604	0.00000	0.773604
0.00506	0.773938	0.00586	0.774117
0.00819	0.774146	0.00768	0.774280
0.01084	0.774338	0.00968	0.774468
0.01249	0.774445	0.01039	0.774527
0.01805	0.774898	0.01558	0.775074
0.02315	0.775300	0.01983	0.775512
0.02526	0.775459	0.02446	0.776001
0.04972	0.777651	0.04850	0.778780
0.07448	0.780070	0.07321	0.781808
0.09480	0.782145	0.09832	0.784942
iC$_4$E$_1$		tC$_4$E$_1$	
x_2	ρ / g cm^{-3}	x_2	ρ / g cm^{-3}
0.00000	0.773604	0.00000	0.773604
0.00510	0.774013	0.00581	0.774096
0.00850	0.774266	0.00775	0.774274
0.01202	0.774569	0.01012	0.774496
0.01576	0.774949	0.01108	0.774574
0.02029	0.775324	0.01709	0.775174
0.02374	0.775683	0.02191	0.775661
0.04785	0.778222	0.02452	0.775914
0.07418	0.781236	0.04819	0.778518
0.09774	0.783958	0.07219	0.781335
		0.09557	0.784131

TABLE S2 Relative permittivity ε_r and apparent dipole moment μ_s calculated by Fröhlich's eqn (7) and (19), and by OKFm eqn (11) and (21) of 1-propoxypropan-2-ol (1-pp-2-ol), 2-butoxyethanol (nC$_4$E$_1$), 2-isobutoxyethanol (iC$_4$E$_1$) and 2-*tert*-butoxyethanol (tC$_4$E$_1$) at different mole fractions x_2 in cyclohexane at T = 298.15 K

x_2	ε_r	μ_s (Fröhlich)/D		μ_s (OKFm)/D	
		eqn (19)	eqn (7)	eqn (21)	eqn (11)
		1-pp-2-ol			
0.0000664	2.01686	2.118	2.202	2.138	2.221
0.0002346	2.01767	2.118	2.150	2.138	2.168
0.0004094	2.01848	2.118	2.127	2.138	2.145
0.000755	2.02012	2.118	2.123	2.138	2.141
0.002853	2.03014	2.116	2.122	2.135	2.140
0.004230	2.03666	2.114	2.118	2.134	2.137
0.005505	2.04270	2.113	2.117	2.132	2.135
0.006935	2.04945	2.112	2.114	2.131	2.132
0.008152	2.05518	2.111	2.112	2.130	2.130
0.009299	2.06062	2.109	2.111	2.128	2.130
0.010457	2.06605	2.108	2.109	2.127	2.128
0.013326	2.07947	2.105	2.105	2.124	2.124
0.016113	2.09243	2.102	2.101	2.121	2.120
0.018841	2.10515	2.100	2.098	2.118	2.117
0.021592	2.11808	2.097	2.096	2.115	2.115
0.024339	2.13082	2.093	2.093	2.112	2.112
0.027042	2.14333	2.090	2.090	2.110	2.110
0.029757	2.15587	2.087	2.088	2.138	2.107
0.040801	2.20557		2.072		2.092
0.050685	2.25091		2.065		2.086
0.060839	2.29749		2.060		2.081
0.072029	2.34894		2.055		2.076
0.081621	2.39345		2.052		2.073
0.091097	2.43761		2.049		2.071
		nC$_4$E$_1$			
0.0000447	2.01670	2.110	1.948	2.134	1.969
0.0002117	2.01750	2.109	2.082	2.134	2.104
0.0003824	2.01830	2.109	2.085	2.134	2.106
0.0007459	2.02002	2.108	2.093	2.133	2.115
0.0014562	2.02341	2.107	2.102	2.132	2.124
0.0026740	2.02920	2.105	2.104	2.129	2.126
0.0039530	2.03530	2.103	2.106	2.127	2.128
0.0048593	2.03970	2.101	2.110	2.125	2.132
0.006448	2.04709	2.098	2.102	2.122	2.125
0.008023	2.05447	2.096	2.099	2.119	2.121
0.009725	2.06236	2.092	2.094	2.115	2.116
0.011346	2.06985	2.089	2.090	2.112	2.113
0.012970	2.07732	2.086	2.086	2.109	2.109
0.016173	2.09192	2.080	2.079	2.102	2.101
0.019439	2.10666	2.074	2.072	2.096	2.094
0.022669	2.12113	2.067	2.065	2.089	2.088
0.030414	2.15554	2.051	2.052	2.073	2.074
0.036896	2.18422		2.043		2.066
0.044605	2.21840		2.035		2.058
0.053092	2.25894		2.040		2.064
0.064532	2.30969		2.031		2.054
0.076012	2.36128		2.024		2.048
0.087102	2.41173		2.020		2.044
0.097897	2.46157		2.018		2.042

x_2	ε_r	μ_s (Fröhlich)/D		μ_s (OKFm)/D	
		eqn (19)	eqn (7)	eqn (21)	eqn (11)
			iC$_4$E$_1$		
0.0000819	2.01682	2.062	1.852	2.084	1.869
0.0002455	2.01757	2.062	2.000	2.084	2.019
0.0004260	2.01839	2.062	2.026	2.084	2.045
0.000750	2.01985	2.061	2.041	2.083	2.060
0.001539	2.02341	2.060	2.048	2.082	2.068
0.002806	2.02914	2.059	2.053	2.080	2.073
0.004031	2.03467	2.057	2.054	2.078	2.074
0.005226	2.04011	2.055	2.056	2.076	2.075
0.006804	2.04724	2.053	2.055	2.074	2.075
0.007817	2.05175	2.052	2.053	2.072	2.072
0.010044	2.06167	2.048	2.049	2.068	2.069
0.011881	2.06979	2.046	2.046	2.065	2.065
0.014098	2.07959	2.042	2.042	2.062	2.062
0.017201	2.09320	2.037	2.037	2.057	2.057
0.020148	2.10606	2.033	2.033	2.052	2.052
0.023737	2.12154	2.027	2.026	2.046	2.046
0.030354	2.14977	2.015	2.015	2.035	2.035
0.045449	2.21374		1.997		2.018
0.053976	2.25161		1.998		2.018
0.065289	2.29997		1.990		2.011
0.076346	2.34775		1.985		2.006
0.087005	2.39437		1.982		2.003
			tC$_4$E$_1$		
0.0000791	2.01704	2.279	2.502	2.305	2.526
0.0002413	2.01794	2.279	2.356	2.305	2.379
0.0004069	2.01886	2.278	2.332	2.304	2.355
0.0007266	2.02064	2.278	2.313	2.303	2.335
0.001677	2.02586	2.275	2.291	2.301	2.313
0.002946	2.03284	2.272	2.284	2.297	2.306
0.004237	2.03988	2.269	2.277	2.293	2.300
0.005096	2.04452	2.266	2.273	2.290	2.295
0.006778	2.05353	2.262	2.265	2.285	2.287
0.008274	2.06153	2.258	2.259	2.281	2.281
0.009937	2.07046	2.253	2.255	2.276	2.278
0.011419	2.07827	2.249	2.250	2.272	2.272
0.012976	2.08642	2.245	2.245	2.267	2.267
0.016084	2.10255	2.236	2.235	2.258	2.257
0.019152	2.11823	2.227	2.225	2.248	2.246
0.022228	2.13381	2.218	2.215	2.239	2.237
0.030150	2.17332	2.193	2.195	2.215	2.216
0.036010	2.20227		2.183		2.204
0.045589	2.24907		2.166		2.186
0.053994	2.29456		2.171		2.192
0.065214	2.34852		2.154		2.174
0.076332	2.40192		2.140		2.160
0.087047	2.45379		2.131		2.150
0.097761	2.50792		2.127		2.146

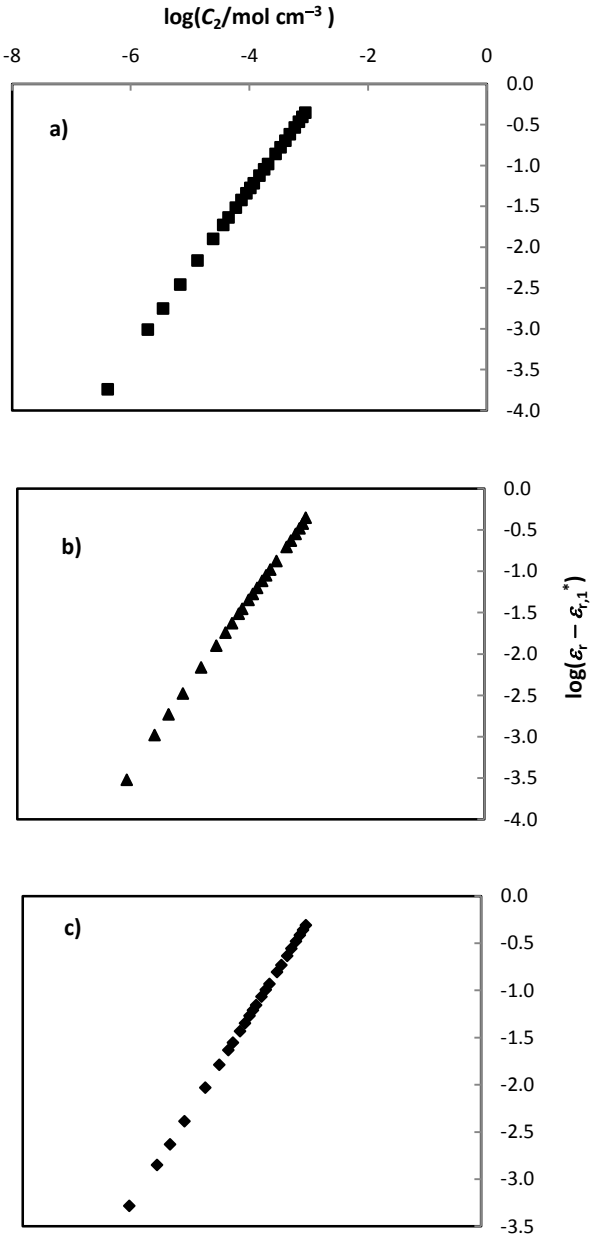

Fig. S1 Log-log plots of increments in relative permittivity, $\varepsilon_r - \varepsilon_{r1}^*$, against solute concentration, C_2, for solutions in cyclohexane at 298.15 K of : (a) *n*C4E1; (b), *i*C4E1; and (c), *t*C4E1.