Journal of the Serbian Chemical Society
JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 78 (9) S110–S116 (2013)
Supplementary material

SUPPLEMENTARY MATERIAL TO

Thermophysical properties of binary mixtures of *N*,*N*-dimethylformamide with three cyclic ethers

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J. Serb. Chem. Soc. 78 (9) (2013) 1443–1460

TABLE S-I. Densities (ρ), viscosities (η), excess molar volumes (V_m^E), excess viscosities (η^E) for the binary mixtures of DMF (1) with the three cyclic ethers (2) at 298.15, 308.15 and 318.15 K; x_1 – mole fraction of DMF

x_1	$\rho\times10^{-3}$ / kg m^{-3}	η / mPa s	$V_m^E\times10^6$ / m^3 mol^{-1}	η^E / mPa s
		DMF (1) + THF (2)		
		T = 298.15 K		
0	0.8807	0.463	0	0
0.0988	0.8873	0.470	–0.058	–0.019
0.1978	0.8938	0.482	–0.099	–0.034
0.2971	0.9003	0.496	–0.131	–0.049
0.3967	0.9067	0.518	–0.146	–0.058
0.4966	0.9131	0.547	–0.153	–0.062
0.5967	0.9193	0.586	–0.135	–0.057
0.6971	0.9254	0.630	–0.101	–0.050
0.7978	0.9315	0.679	–0.061	–0.039
0.8988	0.9377	0.737	–0.021	–0.022
1	0.9442	0.803	0	0
		T = 308.15 K		
0	0.8712	0.428	0	0
0.0988	0.8779	0.434	–0.067	–0.016
0.1978	0.8845	0.444	–0.115	–0.029
0.2971	0.8910	0.458	–0.145	–0.039
0.3967	0.8975	0.476	–0.167	–0.047
0.4966	0.9039	0.502	–0.172	–0.048
0.5967	0.9102	0.533	–0.159	–0.045

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TABLE S-I. Continued

x_1	$\rho\times10^{-3}$ / kg m^{-3}	η / mPa s	$V_m^E\times10^6$ / m^3 mol^{-1}	η^E / mPa s
		DMF (1) + THF (2)		
		T = 308.15 K		
0.6971	0.9164	0.570	–0.130	–0.038
0.7978	0.9227	0.614	–0.103	–0.026
0.8988	0.9289	0.659	–0.059	–0.015
1	0.9350	0.709	0	0
		T = 318.15 K		
0	0.8614	0.390	0	0
0.0988	0.8680	0.410	–0.054	0.002
0.1978	0.8749	0.431	–0.127	0.004
0.2971	0.8817	0.454	–0.181	0.007
0.3967	0.8885	0.478	–0.225	0.010
0.4966	0.8951	0.502	–0.242	0.012
0.5967	0.9013	0.523	–0.214	0.010
0.6971	0.9073	0.545	–0.160	0.008
0.7978	0.9134	0.568	–0.108	0.006
0.8988	0.9195	0.592	–0.049	0.003
1	0.9258	0.617	0	0
		DMF (1) + 1,3-DO (2)		
		T = 298.15 K		
0	1.0571	0.588	0	0
0.1012	1.0454	0.567	–0.053	–0.040
0.2021	1.0338	0.568	–0.096	–0.058
0.3028	1.0222	0.578	–0.121	–0.068
0.4032	1.0106	0.594	–0.127	–0.073
0.5033	0.9991	0.614	–0.120	–0.074
0.6032	0.9876	0.642	–0.095	–0.068
0.7028	0.9764	0.676	–0.073	–0.056
0.8021	0.9654	0.715	–0.046	–0.040
0.9012	0.9546	0.759	–0.017	–0.020
1	0.9442	0.803	0	0.
		T = 308.15 K		
0	1.0459	0.513	0	0
0.1012	1.0345	0.506	–0.059	–0.024
0.2021	1.0232	0.510	–0.108	–0.038
0.3028	1.0119	0.520	–0.140	–0.046
0.4032	1.0006	0.535	–0.153	–0.049
0.5033	0.9895	0.552	–0.162	–0.052
0.6032	0.9783	0.578	–0.145	–0.046
0.7028	0.9673	0.606	–0.124	–0.038
0.8021	0.9564	0.637	–0.091	–0.028
0.9012	0.9456	0.671	–0.047	–0.016
1	0.9350	0.709	0	0

TABLE S-I. Continued

x_1	$\rho\times10^{-3}$ / kg m^{-3}	η / mPa s	$V_m^E\times10^6$ / m^3 mol^{-1}	η^E / mPa s
DMF (1) + 1,3-DO (2)				
T = 318.15 K				
0	1.0334	0.458	0	0
0.1012	1.0221	0.467	–0.040	–0.005
0.2021	1.0115	0.477	–0.114	–0.009
0.3028	1.0008	0.488	–0.164	–0.013
0.4032	0.9901	0.500	–0.196	–0.016
0.5033	0.9793	0.515	–0.204	–0.017
0.6032	0.9683	0.534	–0.178	–0.014
0.7028	0.9573	0.555	–0.132	–0.010
0.8021	0.9466	0.576	–0.091	–0.006
0.9012	0.9359	0.597	–0.030	–0.002
1	0.9258	0.617	0	0
DMF (1) + 1,4-DO (2)				
T = 298.15 K				
0	1.0265	1.196	0	0
0.1181	1.0173	1.109	0.028	–0.032
0.2316	1.0082	1.043	0.059	–0.048
0.3406	0.9992	0.984	0.095	–0.060
0.4455	0.9904	0.934	0.126	–0.067
0.5465	0.9820	0.891	0.135	–0.071
0.6439	0.9739	0.859	0.131	–0.066
0.7377	0.9661	0.835	0.113	–0.056
0.8282	0.9586	0.820	0.081	–0.040
0.9156	0.9513	0.811	0.044	–0.019
1	0.9442	0.803	0	0
T = 308.15 K				
0	1.0166	1.013	0	0
0.1181	1.0077	0.952	0.009	–0.019
0.2316	0.9988	0.899	0.030	–0.034
0.3406	0.9902	0.849	0.039	–0.048
0.4455	0.9817	0.807	0.052	–0.057
0.5465	0.9735	0.772	0.050	–0.061
0.6439	0.9654	0.746	0.052	–0.059
0.7377	0.9576	0.726	0.039	–0.053
0.8282	0.9499	0.714	0.030	–0.040
0.9156	0.9424	0.708	0.014	–0.023
1	0.9350	0.709	0	0
T = 318.15 K				
0	1.0052	0.887	0	0
0.1181	0.9968	0.843	–0.013	–0.007
0.2316	0.9886	0.797	–0.031	–0.018
0.3406	0.9804	0.753	–0.036	–0.031

TABLE S-I. Continued

x_1	$\rho\times10^{-3}$ / kg m^{-3}	η / mPa s	$V_m^E\times10^6$ / m^3 mol^{-1}	η^E / mPa s
		DMF (1) + 1,4-DO (2)		
		T = 318.15 K		
0.4455	0.9724	0.713	–0.046	–0.042
0.5465	0.9644	0.680	–0.045	–0.047
0.6439	0.9564	0.653	–0.034	–0.049
0.7377	0.9486	0.636	–0.028	–0.043
0.8282	0.9408	0.624	–0.012	–0.033
0.9156	0.9332	0.618	–0.002	–0.018
1	0.9258	0.617	0	0

TABLE S-II. Redlich–Kister coefficients (a_k), standard deviations (SD) for the least squares fitting of the excess molar volumes (V_m^E), excess partial molar volumes ($\bar{V}_{m,1}^E$ and $\bar{V}_{m,2}^E$) and these ($\bar{V}_{m,1}^{0,E}$ and $\bar{V}_{m,2}^{0,E}$) at infinite dilution ($\bar{V}_{m,1}^{0,E}$ and $\bar{V}_{m,2}^{0,E}$) of each component in the studied binary mixtures at T = (298.15, 308.15 and 318.15) K; molar volumes are given in cm^3 mol^{-1}

Parameter	DMF (1) +		
	THF (2)	1,3-DO (2)	1,4-DO (2)
	T = 298.15 K		
a_0	–0.596	–0.480	0.520
a_1	0.145	0.290	0.238
a_2	0.251	0.133	–0.180
a_3	0.184	–0.077	–0.058
SD	0.002	0.002	0.003
$\bar{V}_{m,1}^E$	76.75	76.86	77.58
$\bar{V}_{m,2}^E$	81.86	69.94	86.35
$\bar{V}_{m,1}^{0,E}$	–0.674	–0.560	0.160
$\bar{V}_{m,2}^{0,E}$	–0.016	–0.134	0.520
	T = 308.15 K		
a_0	–0.669	–0.637	0.212
a_1	0.097	0.086	0.041
a_2	–0.040	0.068	–0.119
a_3	–0.053	–0.016	0.040
SD	0.004	0.003	0.003
$\bar{V}_{m,1}^E$	77.43	77.54	78.19
$\bar{V}_{m,2}^E$	82.11	70.33	86.84
$\bar{V}_{m,1}^{0,E}$	–0.753	–0.639	0.012
$\bar{V}_{m,2}^{0,E}$	–0.665	–0.499	0.174
	T = 318.15 K		
a_0	–0.933	–0.819	–0.182
a_1	0.177	0.190	0.023
a_2	0.568	0.635	0.155
a_3	–0.203	–0.205	0.048
SD	0.006	0.006	0.003
$\bar{V}_{m,1}^E$	78.62	78.79	78.86

TABLE S-II. Continued

Parameter	DMF (1) +		
	THF (2)	1,3-DO (2)	1,4-DO (2)
	T = 318.15 K		
$\bar{V}^{E}_{m,2}$	83.32	71.49	87.70
$\bar{V}^{0,E}_{m,1}$	–0.339	–0.169	–0.098
$\bar{V}^{0,E}_{m,2}$	–0.391	–0.199	0.044

TABLE S-III. Values of enthalpy (ΔH^*) and entropy (ΔS^*) of activation of viscous flow for the binary mixtures; x_1 – mole fraction of DMF

x_1	ΔH^* / kJ mol^{-1}	ΔS^* / J K^{-1} mol^{-1}	R^2
	DMF (1) + THF (2)		
0	5.884	–18.150	0.9948
0.0988	4.527	–22.725	0.9902
0.1978	3.588	–25.992	0.9089
0.2971	2.695	–29.152	0.7474
0.3967	2.406	–30.410	0.5981
0.4966	2.636	–30.051	0.6587
0.5967	3.736	–26.902	0.8361
0.6971	4.958	–23.390	0.9473
0.7978	6.273	–19.605	0.9956
0.8988	7.865	–14.926	0.9999
1	9.604	–9.790	0.9972
	DMF (1) + 1,3-DO (2)		
0	8.965	–8.460	0.9981
0.1012	6.775	–15.570	0.9902
0.2021	6.041	–18.118	0.9809
0.3028	5.856	–18.963	0.9783
0.4032	5.999	–18.804	0.9849
0.5033	6.158	–18.629	0.9856
0.6032	6.494	–17.973	0.9944
0.7028	7.005	–16.778	0.9971
0.8021	7.753	–16.830	0.9992
0.9012	8.687	–12.288	1.0000
1	9.604	–9.790	0.9972
	DMF (1) + 1,4-DO (2)		
0	10.970	–9.314	0.9971
0.1181	10.022	–11.775	0.9970
0.2316	9.842	–11.781	0.9977
0.3406	9.810	–11.317	0.9978
0.4455	9.929	–10.405	0.9988
0.5465	9.947	–9.876	0.9996
0.6439	10.097	–8.997	1.0000
0.7377	10.014	–8.957	1.0000
0.8282	10.030	–8.673	0.9999

TABLE S-III. Continued

x_1	ΔH^* / kJ mol^{-1}	ΔS^* / J K^{-1} mol^{-1}	R^2
	DMF (1) + 1,4-DO (2)		
0.9156	9.956	–8.754	0.9997
1	9.604	–9.790	0.9972

TABLE S-IV. Ultrasonic speeds (u), isentropic compressibilities (κ_S) and excess isentropic compressibilities (κ_S^E) of binary mixtures of DMF (1) + the cyclic ethers (2) at 298.15 K; x_1 – mole fraction of DMF; x_1 – mole fraction of DMF

x_1	u / m s^{-1}	κ_S×10^{10} / Pa^{-1}	κ_S^E ×10^{10} / Pa^{-1}
	DMF (1) + THF (2)		
0	1277.8	6.954	0
0.0988	1313.2	6.535	–0.254
0.1978	1343.8	5.196	–0.420
0.2971	1369.6	5.921	–0.513
0.3967	1395.5	5.663	–0.581
0.4966	1418.8	5.441	–0.605
0.5967	1438.1	5.260	–0.580
0.6971	1452.1	5.125	–0.500
0.7978	1462.9	5.016	–0.387
0.8988	1463.5	4.979	–0.194
1	1464.8	4.936	0
	DMF (1) + 1,3-DO (2)		
0	1338.2	5.283	0
0.1012	1352.6	5.229	–0.028
0.2021	1369.8	5.155	–0.072
0.3028	1387.8	5.079	–0.117
0.4032	1406.2	5.004	–0.159
0.5033	1424.9	4.930	–0.199
0.6032	1440.4	4.880	–0.212
0.7028	1452.3	4.856	–0.199
0.8021	1460.2	4.858	–0.158
0.9012	1462.8	4.896	–0.082
1	1464.8	4.936	0
	DMF (1) + 1,4-DO (2)		
0	1343.4	5.398	0
0.1181	1368.4	5.250	–0.103
0.2316	1386.5	5.160	–0.148
0.3406	1397.5	5.124	–0.137
0.4455	1404.8	5.116	–0.099
0.5465	1408.6	5.132	–0.036
0.6439	1414.5	5.122	0.010
0.7377	1422.7	5.076	0.038
0.8282	1432.7	5.029	0.053
0.9156	1446.9	4.983	0.039
1	1464.8	4.936	0

TABLE S-V. Relative predictive capabilities of various theories and empirical relations for ultrasonic speeds of the binary mixtures at 298.15 K

DMF (1) +	*MRSD*[a] / %				
	FLORY	CFT	NOM	IMR	IDR
THF (2)	1.96	2.50	2.86	3.15	2.43
1,3-DO (2)	1.48	1.10	1.10	1.40	1.39
1,4-DO (2)	1.74	0.70	0.76	0.76	0.72

[a] $MRSD = 100\left[\frac{1}{N}\sum\{(u_{\text{exp}} - u_{\text{cal}})/u_{\text{exp}}\}^2\right]^{1/2}$; *N* is number of data points

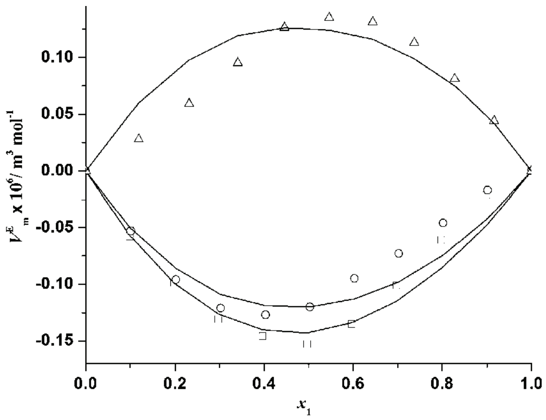

Fig. S-1. Comparison between the experimental excess molar volumes and the excess molar volumes obtained from the Prigogine–Flory–Patterson theory as a function of the mole fraction of DMF (x_1) for binary mixtures of DMF with cyclic ethers at T = 298.15 K. The graphical points represent the experimental excess molar volumes ($V^{\text{E}}_{\text{m,exp}}$): □, THF; ○, 1,3-DO; Δ, 1,4-DO and the smooth curves represent the $V^{\text{E}}_{\text{m,PFP}}$ values obtained from the Prigogine–Flory–Patterson theory.

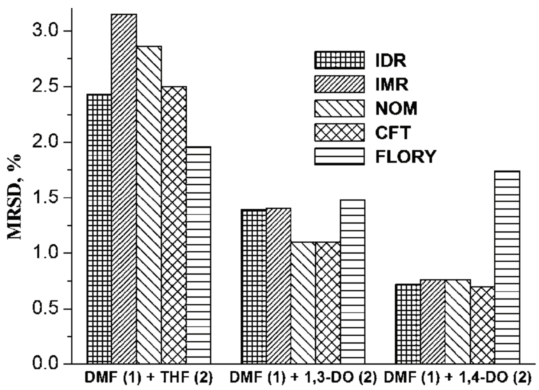

Fig. S-2. MRSD values for the theoretical prediction of the ultrasonic speeds by different theories and empirical relations for the binary mixtures of DMF + cyclic ethers at T = 298.15 K.