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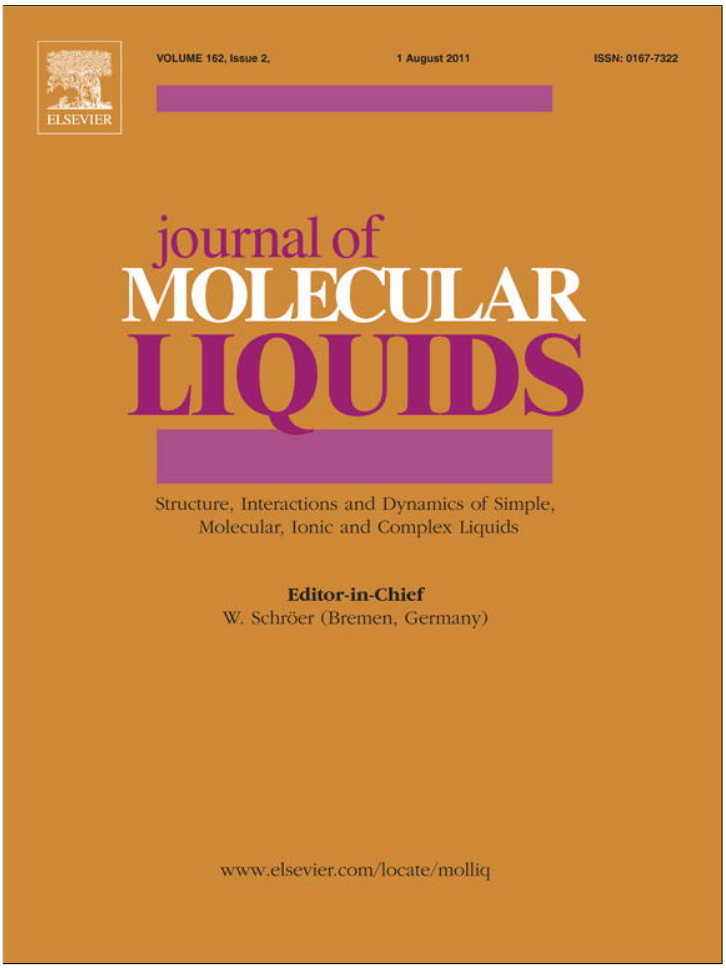

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Prediction of viscosity of binary solvent mixtures at various temperatures

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ABSTRACT

Combined forms of the Jouyban–Acree model and the calculated Abraham solute parameters as descriptors for solvents were used for predicting the viscosity of binary solvent mixtures at various temperatures. The proposed models were tested on a large number of the experimental data of binary miscible mixtures. The mean relative deviations (MRDs) between computed and experimental viscosity data are used as an accuracy criterion. The overall MRD for the investigated mixtures is 17%. With including the experimental viscosity of mono-solvents, the prediction capability of the proposed model is improved and the overall MRD is 7%. A reduced form of the model could be used to compute the viscosity of mono-solvents at various temperatures with the MRD of 27%.

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1. Introduction

Viscosity is an expression of the resistance of a fluid to flow, and the knowledge of viscosity of mono-solvents and solvent mixtures at various temperatures is required in many industrial applications. Despite of the reported experimental viscosity data for mixed solvents at ambient or various temperatures in the chemical literature, a number of models have been presented to calculate the viscosity. These include the Arrhenius [1], the Grunberg and Nissan [2], the Redlich–Kister [3], and the Jouyban–Acree [4] models. More details of these models and a comprehensive comparison of the accuracies of the models were presented in a previous publication [4]. Among the investigated models, the Jouyban–Acree model provided the most accurate results. The model requires the experimental viscosities in mono-solvents and a number of viscosity data in mixed solvents to calculate the model constants, and these requirements restrict its practical applications. The aims of this work are to propose extended versions of the model to predict the viscosity of binary solvent mixtures at various temperatures using a minimum number of experimental data and also an ab initio prediction method.

2. Experimental

2.1. Computational methods

The Jouyban–Acree model for calculating the viscosity of binary solvents at various temperatures is:

$$\ln \eta_{m,T} = x_1 \ln \eta_{1,T} + x_2 \ln \eta_{2,T} + J_0\left[\frac{x_1 x_2}{T}\right] + J_1\left[\frac{x_1 x_2 (x_1 - x_2)}{T}\right] + J_2\left[\frac{x_1 x_2 (x_1 - x_2)^2}{T}\right] \quad (1)$$

where $\eta_{m,T}$, $\eta_{1,T}$ and $\eta_{2,T}$ are viscosity of mixed solvents and pure solvents 1 and 2 at temperature T, x_1 and x_2 are the fractions of the solvents 1 and 2, and $J_0 - J_2$ are the model constants. These constants are computed by a least squares analysis [4].

In order to provide more comprehensive model, it is possible to include physico-chemical properties of the solvents affecting the viscosity of a given binary mixture. Abraham and co-workers proposed the linear free energy relationship (LFER) equations to calculate various physico-chemical properties (*PP*) as [5]

$$\log PP = c + eE + sS + aA + bB + vV \quad (2)$$

in which c, e, s, a, b and v are the model constants which are indicators of solvent (or system) properties, E is the excess molar refraction, S is dipolarity/polarizability of the analyte, A denotes the analyte's hydrogen-bond acidity, B stands for the analyte's hydrogen-bond basicity and V is the McGowan volume of the analytes (for the

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Table 1
List of solvents in this study along their related calculated Abraham solute parameters.

Solvent	E	S	A	B	V
(S)-(-)-Limonene	0.450	0.320	0.000	0.200	1.323
1-Bromobutane	0.310	0.410	0.000	0.030	0.847
1-Bromopentane	0.310	0.410	0.000	0.040	0.988
1-Bromopropane	0.310	0.400	0.000	0.000	0.706
1-Butanol	0.200	0.460	0.310	0.310	0.731
1-Chlorobutane	0.120	0.320	0.000	0.000	0.796
1-Chloronaphthalene	1.420	1.100	0.000	0.170	1.208
1-Decanol	0.190	0.480	0.310	0.330	1.576
1-Dodecanol	0.190	0.490	0.310	0.340	1.858
1-Heptanol	0.200	0.470	0.310	0.317	1.154
1-Hexanol	0.200	0.460	0.310	0.312	1.013
1-Nonanol	0.200	0.480	0.310	0.330	1.435
1-Octanol	0.200	0.470	0.310	0.317	1.295
1-Pentanol	0.200	0.460	0.310	0.317	0.872
1-Propanol	0.210	0.450	0.310	0.308	0.590
1,1,2,2-Tetrabromoethane	1.360	0.930	0.180	0.120	1.090
1,1,2,2-Tetrachloroethane	0.630	0.600	0.180	0.100	0.880
1,2-Dichloroethane	0.380	0.480	0.000	0.100	0.635
1,3-Dioxolane	0.290	0.570	0.000	0.424	0.540
1,4-Dioxane	0.290	0.580	0.000	0.440	0.681
1,8-Cineole	0.430	0.390	0.000	0.320	1.591
2-Methylpropan-2-ol	0.190	0.390	0.310	0.350	0.731
2-(2-Methoxyethoxy)ethanol	0.320	0.710	0.230	0.830	0.989
2-[2-(2-Methoxyethoxy)ethoxy]ethanol	0.360	0.870	0.230	1.050	1.330
2-Butanol	0.210	0.440	0.310	0.339	0.731
2-Butanone	0.220	0.670	0.000	0.300	0.688
2-Chlorobutane	0.130	0.310	0.000	0.100	0.795
2-Chloroethanol	0.330	0.590	0.380	0.310	0.572
2-Heptanol	0.210	0.450	0.310	0.350	1.154
2-Hexanol	0.210	0.450	0.310	0.350	1.013
2-Methoxyethanol	0.280	0.540	0.230	0.620	0.649
2-Methyl-1-propanol	0.210	0.440	0.310	0.340	0.731
2-Methyl-1-propanol	0.210	0.440	0.310	0.340	0.731
2-Methyl-2-butanol	0.190	0.390	0.310	0.350	0.872
2-Methyl-2-chloropropane	0.110	0.260	0.000	0.100	0.795
2-Octanol	0.210	0.460	0.310	0.350	1.295
2-Pentanol	0.210	0.440	0.310	0.340	0.872
2-Pentanone	0.210	0.680	0.000	0.300	0.829
2-Propanol	0.220	0.430	0.310	0.340	0.590
2-Propanol	0.220	0.430	0.310	0.340	0.590
2,2,4-Trimethylpentane	−0.010	0.120	0.000	0.100	1.236
3-Methyl-1-butanol	0.210	0.440	0.310	0.340	0.872
Acetone	0.220	0.670	0.000	0.300	0.547
Acetonitrile	0.190	0.720	0.000	0.200	0.404
Acetophenone	0.790	1.130	0.000	0.400	1.014
Acrylonitrile	0.310	0.780	0.000	0.300	0.502
alfa-Pinene	0.550	0.330	0.000	0.180	1.257
Aniline	0.860	1.080	0.230	0.430	0.816
Anisole	0.620	0.790	0.000	0.313	0.916
Benzene	0.560	0.690	0.000	0.106	0.716
Benzonitrile	0.730	1.170	0.000	0.280	0.871
Benzoyl chloride	0.910	1.270	0.000	0.420	0.995
Benzyl alcohol	0.800	0.840	0.310	0.530	0.916
beta-Pinene	0.520	0.280	0.000	0.160	1.257
Bromobenzene	0.890	0.850	0.000	0.110	0.891
Bromoform	0.880	0.730	0.120	0.010	0.775
Butyl acetate	0.060	0.590	0.000	0.390	1.028
Butylamine	0.200	0.500	0.210	0.597	0.772
Chlorobenzene	0.700	0.770	0.000	0.110	0.839
Chloroform	0.340	0.480	0.120	0.000	0.617
Cyclohexane	0.210	0.280	0.000	0.013	0.845
Cyclohexanol	0.420	0.530	0.310	0.320	0.904
Decane	−0.010	0.210	0.000	0.100	1.518
Di-n-butylamine	0.150	0.370	0.130	0.490	1.336
Dibutyl ether	0.040	0.350	0.000	0.260	1.295
Dimethoxyethane	0.090	0.480	0.000	0.500	0.790
Dimethylformamide	0.350	1.110	0.000	0.629	0.647
Dimethysulfoxide	0.520	1.370	0.000	0.710	0.613
N,N-Dimethylacetamide	0.330	1.060	0.000	0.640	0.788
Dodecane	−0.010	0.220	0.000	0.080	1.799
Ethanol	0.210	0.450	0.310	0.308	0.449
Ethenylbenzene	0.700	0.700	0.000	0.190	0.955
Ethyl acetate	0.070	0.580	0.000	0.383	0.747
Ethyl tert-butyl ether	0.020	0.280	0.000	0.300	1.013
Ethylene glycol	0.410	0.710	0.540	0.580	0.508

(*continued on next page*)

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Table 1 (*continued*)

Solvent	E	S	A	B	V
Ethylether	0.040	0.340	0.000	0.300	0.731
Formamid	0.450	1.140	0.490	0.560	0.365
Glycerol	0.610	0.970	0.810	0.890	0.707
Heptane	0.000	0.200	0.000	0.100	1.095
Hexane	0.000	0.190	0.000	0.000	0.954
m-Cresol	0.810	0.850	0.500	0.393	0.916
m-Xylene	0.610	0.580	0.000	0.106	0.998
Mesitylene	0.630	0.520	0.000	0.106	1.139
Methanol	0.210	0.440	0.310	0.300	0.308
Methyl acetate	0.070	0.570	0.000	0.390	0.606
Methylcyclohexane	0.220	0.270	0.000	0.073	0.986
Methylcyclopentane	0.220	0.260	0.000	0.050	0.845
N-Methylacetamide	0.320	1.050	0.260	0.590	0.647
Nitrobenzene	0.830	1.260	0.000	0.210	0.891
Nitromethane	0.230	0.710	0.000	0.220	0.424
Nonane	−0.010	0.200	0.000	0.100	1.377
o-Cresol	0.810	0.850	0.500	0.393	0.916
o-Xylene	0.610	0.580	0.000	0.106	0.998
Octane	0.000	0.200	0.000	0.100	1.236
p-Cresol	0.810	0.850	0.500	0.390	0.916
p-Cymene	0.610	0.570	0.000	0.150	1.280
p-Xylene	0.610	0.580	0.000	0.108	0.998
Propiophenone	0.790	1.140	0.000	0.400	1.155
Propyl acetate	0.070	0.580	0.000	0.390	0.888
Propylbenzene	0.580	0.640	0.000	0.120	1.139
Propylene glycol monoethyl ether	0.790	1.140	0.000	0.400	1.155
Propylene glycol monomethyl ether	0.790	1.140	0.000	0.400	1.155
Propylene glycol monopropyl ether	0.790	1.140	0.000	0.400	1.155
Propylene glycol tert-butyl ether	0.790	1.140	0.000	0.430	1.155
Pyridine	0.600	0.820	0.000	0.400	0.675
tert-Amyl methyl ether	0.020	0.280	0.000	0.300	1.013
tert-Butyl methyl ether	0.020	0.270	0.000	0.300	0.872
Tetrachloromethane	0.420	0.550	0.000	0.000	0.739
Tetrahydrofuran	0.250	0.420	0.000	0.200	0.622
Toluene	0.560	0.630	0.000	0.108	0.857
Tri-n-butylamine	0.160	0.400	0.000	0.595	1.899
Trichloroethane	0.310	0.440	0.000	0.000	0.758
Trichloroethylene	0.500	0.640	0.000	0.100	0.715
Triethylamine	0.170	0.370	0.000	0.500	1.054

numerical values of these parameters see Table 1). The numerical values of *c*, *e*, *s*, *a*, *b* and *v* terms are not available for some solvents and there is no available software to compute these parameters, however, the numerical values of *E*, *S*, *A*, *B* and *V* could be calculated using Pharma-Algorithms software [6]. In treating the solute–solvent interactions, both parameters are required, but in the case of physico-chemical properties of two solvents in the absence of any solute, the solute parameters of Abraham could also be employed to represent the interactions between two solvents in the mixtures. Therefore, J_i terms of Eq. (1) which are due to the various solvent–solvent interactions in the solution [7], could be represented by Abraham solute parameters and Eq. (1) could be re-written as

$$\begin{aligned} ln\,\eta_{m,T} = {} & x_1\,ln\,\eta_{1,T} + x_2\,ln\,\eta_{2,T} + \frac{x_1x_2}{T}[W_0 + W_1(E_1-E_2)^2 \\ & + W_2(S_1-S_2)^2 + W_3(A_1-A_2)^2 + W_4(B_1-B_2)^2 \\ & + W_5(V_1-V_2)^2] + \frac{x_1x_2(x_1-x_2)}{T}[W_0' + W_1'(E_1-E_2)^2 \\ & + W_2'(S_1-S_2)^2 + W_3'(A_1-A_2)^2 + W_4'(B_1-B_2)^2(V_1-V_2)^2] \\ & + \frac{x_1x_2(x_1-x_2)^2}{T}[W_0'' + W_1''(E_1-E_2)^2 + W_2''(S_1-S_2)^2 \\ & + W_3''(A_1-A_2)^2 + W_4''(B_1-B_2)^2 + W_5''(V_1-V_2)^2] \end{aligned} \quad (3)$$

where subscripts 1 and 2 are the properties of solvents 1 and 2, and *W* terms are the model constants representing the two and three body interaction energies of the solvents. From a mathematical point of view, they are adjustable curve-fit parameters determined from regressing $(\ln \eta_{m,T} - x_1 \ln \eta_{1,T} - x_2 \ln \eta_{2,T})$ against $\frac{x_1x_2}{T}$, $\frac{x_1x_2(E_1-E_2)^2}{T}$, $\frac{x_1x_2(S_1-S_2)^2}{T}$, $\frac{x_1x_2(A_1-A_2)^2}{T}$, $\frac{x_1x_2(B_1-B_2)^2}{T}$, $\frac{x_1x_2(V_1-V_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)}{T}$, $\frac{x_1x_2(x_1-x_2)(E_1-E_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)(S_1-S_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)(A_1-A_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)(B_1-B_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)(V_1-V_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)^2(E_1-E_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)^2(S_1-S_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)^2(A_1-A_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)^2(B_1-B_2)^2}{T}$ and $\frac{x_1x_2(x_1-x_2)^2(V_1-V_2)^2}{T}$ using a no intercept least square analysis. The Abraham solvation parameters account for possible interactions between solvents 1 and 2 in the mixture. The model can be used to predict the viscosity of different binary mixtures at various temperatures by employing the corresponding experimental η_1 and η_2 values of the mono-solvents at *T*.

The number of experimental data points required in the computation process of η_m, can be reduced by considering a

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Table 2
List of solvent mixtures studied in this work, temperature (*T*), number of data points (*N*), MRDs and d_{rms} of Eqs. (6) and (7).

No.	Solvent 1	Solvent 2	T/K	Ref	N	MRD Eq. (6)	MRD Eq. (7)	d_{rms} Eq. (6)	d_{rms} Eq. (7)
1	(S)-(-)-Limonene	Hexane	298	[8]	14	1	27	0.1	2.3
2	1-Bromobutane	1, 4-Dimethylbenzene	308	[9]	11	1	5	0.1	0.5
3	1-Bromobutane	Benzene	308	[9]	11	1	4	0.1	0.4
4	1-Bromopentane	1, 3, 5-Trimethylbenzene	308	[9]	11	2	6	0.2	0.6
5	1-Bromobutane	1, 4-Dimethylbenzene	308	[9]	11	1	6	0.1	0.6
6	1-Bromobutane	Benzene	308	[9]	11	1	5	0.1	0.5
7	1-Butanol	Acrylonitrile	298	[10]	11	4	10	0.4	0.9
8	1-Butanol	Acrylonitrile	303	[10]	11	4	8	0.4	0.7
9	1-Butanol	Acrylonitrile	308	[10]	11	3	6	0.3	0.6
10	1-Butanol	Anisole	298	[11]	11	9	8	0.8	0.9
11	1-Butanol	Anisole	303	[11]	11	8	8	0.8	0.9
12	1-Butanol	Anisole	308	[11]	11	8	8	0.7	0.9
13	1-Butanol	Benzonitrile	303	[12]	11	2	6	0.2	0.6
14	1-Butanol	Benzonitrile	308	[12]	11	2	6	0.2	0.6
15	1-Butanol	Butylamine	293	[13]	11	28	25	3.4	2.8
16	1-Butanol	Butylamine	303	[13]	11	25	25	3.1	2.8
17	1-Butanol	Butylamine	313	[13]	11	24	25	2.8	2.8
18	1-Butanol	Chloroform	313	[14]	21	3	4	0.3	0.4
19	1-Butanol	Cyclohexane	303	[15]	11	3	22	0.3	2.7
20	1-Butanol	Dimethoxyethane	298	[16]	11	42	45	3.4	3.6
21	1-Butanol	Mesitylene	298	[17]	11	7	24	0.7	2.1
22	1-Butanol	Mesitylene	303	[17]	11	8	23	0.8	2.1
23	1-Butanol	Mesitylene	308	[17]	11	7	21	0.7	1.9
24	1-Butanol	Methylcyclohexane	298	[18]	11	22	29	2.5	3.6
25	1-Butanol	Methylcyclohexane	303	[18]	11	21	29	2.5	3.6
26	1-Butanol	Methylcyclohexane	308	[18]	11	20	28	2.3	3.4
27	1-Butanol	Propylene glycol monoethyl ether	298	[19]	26	12	22	1.3	2.5
28	1-Butanol	Propylene glycol monopropyl ether	298	[19]	25	13	28	1.5	3.5
29	1-Butanol	Toluene	298	[20]	11	6	25	0.6	2.2
30	1-Butanol	Toluene	303	[20]	11	5	21	0.4	1.9
31	1-Butanol	Toluene	308	[20]	11	5	18	0.4	1.6
32	1-Butanol	Toluene	313	[20]	11	4	17	0.4	1.5
33	1-Butanol	Toluene	318	[20]	11	4	10	0.4	1.0
34	1-Butanol	tri-n-Butylamine	303	[21]	11	1	9	0.1	0.9
35	1-Butanol	tri-n-Butylamine	313	[21]	11	3	8	0.3	0.8
36	1-Butanol	Trichloromethane	298	[22]	21	5	9	0.5	0.9
37	1-Butanol	Trichloromethane	308	[22]	21	4	6	0.4	0.5
38	1-Chloronaphthalene	Ethenylbenzene	298	[10]	11	2	3	0.2	0.3
39	1-Chloronaphthalene	Ethenylbenzene	303	[10]	11	2	2	0.2	0.2
40	1-Chloronaphthalene	Ethenylbenzene	308	[10]	11	2	2	0.2	0.2
41	1-Decanol	1,1,2,2-Tetrabromoethane	293	[77]	11	2	21	0.2	1.9
42	1-Decanol	1,1,2,2-Tetrabromoethane	303	[77]	11	3	26	0.3	2.3
43	1-Decanol	Chloroform	298	[14]	21	10	14	1.1	1.6
44	1-Decanol	Chloroform	303	[14]	21	10	12	1.0	1.3
45	1-Decanol	Chloroform	308	[14]	21	9	11	1.0	1.2
46	1-Decanol	Chloroform	313	[14]	21	8	11	0.8	1.2
47	1-Decanol	Cyclohexane	303	[15]	11	13	29	1.4	3.6
48	1-Dodecanol	Cyclohexane	303	[15]	11	17	33	2.0	4.3
49	1-Heptanol	Chloroform	298	[14]	21	6	8	0.6	0.8
50	1-Heptanol	Chloroform	303	[14]	21	5	8	0.5	0.8
51	1-Heptanol	Chloroform	308	[14]	21	4	6	0.4	0.6
52	1-Heptanol	Chloroform	313	[14]	21	4	5	0.4	0.5
53	1-Heptanol	Cyclohexane	303	[15]	11	8	25	0.8	3.0
54	1-Heptanol	Methylcyclohexane	298	[23]	12	7	18	0.7	2.0
55	1-Heptanol	tri-n-Butylamine	303	[15]	11	3	4	0.3	0.4
56	1-Heptanol	tri-n-Butylamine	313	[15]	11	1	5	0.1	0.5
57	1-Heptanol	Trichloroethylene	298	[23]	12	9	9	1.0	0.9
58	1-Hexanol	Chloroform	298	[14]	21	5	8	0.5	0.8
59	1-Hexanol	Chloroform	303	[14]	21	5	7	0.5	0.7
60	1-Hexanol	Chloroform	308	[14]	21	3	5	0.3	0.5
61	1-Hexanol	Chloroform	313	[14]	21	2	3	0.2	0.3
62	1-Hexanol	Cyclohexane	303	[15]	11	6	24	0.7	2.9
63	1-Hexanol	Dimethoxyethane	298	[16]	11	69	71	4.5	4.7
64	1-Nonanol	Cyclohexane	303	[15]	11	13	29	1.4	3.6
65	1-Octanol	1,1,2,2-Tetrachloroethane	298	[24]	16	3	42	0.3	3.1
66	1-Octanol	1,1,2,2-Tetrachloroethane	308	[24]	16	3	38	0.2	2.9
67	1-Octanol	1,2-Dichloroethane	298	[24]	16	10	25	1.0	3.0
68	1-Octanol	1,2-Dichloroethane	308	[24]	16	9	29	0.9	3.6
69	1-Octanol	Chloroform	298	[24]	16	20	22	2.3	2.5
70	1-Octanol	Chloroform	298	[14]	21	7	10	0.7	1.1
71	1-Octanol	Chloroform	303	[14]	21	7	10	0.8	1.1
72	1-Octanol	Chloroform	308	[14]	21	8	10	0.8	1.1

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Table 2 (*continued*)

No.	Solvent 1	Solvent 2	T/K	Ref	N	MRD Eq. (6)	MRD Eq. (7)	d_{rms} Eq. (6)	d_{rms} Eq. (7)
73	1-Octanol	Chloroform	313	[14]	21	6	8	0.6	0.8
74	1-Octanol	Cyclohexane	303	[15]	11	10	29	1.1	3.6
75	1-Octanol	Dimethoxyethane	298	[16]	11	6	6	0.6	0.5
76	1-Octanol	tri-n-Butylamine	303	[21]	11	4	3	0.4	0.3
77	1-Octanol	tri-n-Butylamine	313	[21]	11	2	4	0.2	0.4
78	1-Pentanol	2-Chloroethanol	298	[10]	11	2	12	0.2	1.3
79	1-Pentanol	2-Chloroethanol	303	[10]	11	2	11	0.2	1.2
80	1-Pentanol	2-Chloroethanol	308	[10]	11	2	11	0.3	1.1
81	1-Pentanol	Acrylonitrile	298	[25]	11	2	7	0.2	0.7
82	1-Pentanol	Acrylonitrile	303	[25]	11	3	6	0.2	0.6
83	1-Pentanol	Acrylonitrile	308	[25]	11	3	5	0.2	0.5
84	1-Pentanol	Anisole	298	[11]	11	9	8	0.8	0.8
85	1-Pentanol	Anisole	303	[11]	11	8	8	0.8	0.8
86	1-Pentanol	Anisole	308	[11]	11	8	9	0.7	0.9
87	1-Pentanol	Chloroform	298	[14]	21	4	8	0.4	0.8
88	1-Pentanol	Chloroform	303	[14]	21	4	6	0.4	0.6
89	1-Pentanol	Chloroform	308	[14]	21	3	5	0.3	0.5
90	1-Pentanol	Chloroform	313	[14]	21	3	3	0.3	0.3
91	1-Pentanol	Cyclohexane	303	[15]	11	5	22	0.5	2.6
92	1-Pentanol	Dimethoxyethane	298	[16]	11	56	58	4.0	4.2
93	1-Pentanol	Mesitylene	298	[17]	11	5	23	0.5	2.0
94	1-Pentanol	Mesitylene	303	[17]	11	5	21	0.4	1.9
95	1-Pentanol	Mesitylene	308	[17]	11	5	21	0.5	1.8
96	1-Pentanol	tert-Amyl methyl ether	298	[26]	22	1	8	0.1	0.7
97	1-Pentanol	tert-Butyl methyl ether	298	[26]	23	2	14	0.2	1.3
98	1-Pentanol	Tri-n-Butylamine	303	[21]	11	1	7	0.1	0.7
99	1-Pentanol	tri-n-Butylamine	313	[21]	11	4	6	0.4	0.6
100	1-Propanol	Acrylonitrile	298	[25]	11	7	10	0.7	0.9
101	1-Propanol	Acrylonitrile	303	[25]	11	7	8	0.7	0.8
102	1-Propanol	Acrylonitrile	308	[25]	11	6	6	0.6	0.6
103	1-Propanol	Anisole	298	[11]	11	5	6	0.5	0.6
104	1-Propanol	Anisole	303	[11]	11	7	6	0.6	0.7
105	1-Propanol	Anisole	308	[11]	11	8	7	0.7	0.7
106	1-Propanol	Benzonitrile	303	[12]	11	1	8	0.1	0.9
107	1-Propanol	Benzonitrile	308	[12]	11	1	10	0.1	1.0
108	1-Propanol	Chloroform	313	[14]	21	4	6	0.3	0.6
109	1-Propanol	Cyclohexane	303	[15]	11	2	25	0.2	3.0
110	1-Propanol	Cyclohexane	304	[27]	11	3	25	0.3	3.0
111	1-Propanol	Dimethoxyethane	298	[16]	11	12	10	1.1	0.9
112	1-Propanol	Mesitylene	298	[17]	11	6	23	0.5	2.0
113	1-Propanol	Mesitylene	303	[17]	11	7	20	0.7	1.8
114	1-Propanol	Mesitylene	308	[17]	11	7	18	0.7	1.7
115	1-Propanol	Methylcyclohexane	298	[18]	11	2	15	0.2	1.7
116	1-Propanol	Methylcyclohexane	303	[18]	11	1	16	0.1	1.7
117	1-Propanol	Methylcyclohexane	308	[18]	11	1	16	0.1	1.7
118	1-Propanol	tert-Amyl methyl ether	298	[26]	23	5	9	0.5	0.9
119	1-Propanol	tert-Butyl methyl ether	298	[26]	24	5	16	0.5	1.4
120	1-Propanol	Tetrahydrofuran	293	[28]	12	11	18	1.2	2.0
121	1-Propanol	Tetrahydrofuran	303	[28]	12	9	13	1.0	1.5
122	1-Propanol	Tetrahydrofuran	313	[28]	12	8	17	0.9	1.9
123	1-Propanol	tri-n-Butylamine	303	[21]	11	1	11	0.1	1.2
124	1-Propanol	tri-n-Butylamine	303	[27]	11	2	11	0.2	1.2
125	1-Propanol	tri-n-Butylamine	313	[21]	11	4	10	0.4	1.1
126	1-Propanol	Trichloromethane	298	[22]	21	5	10	0.5	1.0
127	1-Propanol	Trichloromethane	308	[22]	21	4	6	0.3	0.6
128	1-Propanol	Triethylamine	303	[27]	11	5	22	0.5	1.8
129	1, 3, 5-Trimethylbenzene	1-Bromobutane	308	[9]	11	2	19	0.2	1.7
130	1, 3, 5-Trimethylbenzene	1-Bromopropane	308	[9]	11	1	20	0.1	1.7
131	1, 4-Dimethylbenzene	1-Bromopropane	308	[9]	11	2	18	0.2	1.5
132	1,1,2,2-Tetrabromoethane	1-Heptanol	293	[77]	11	0	23	0.0	2.6
133	1,1,2,2-Tetrabromoethane	1-Heptanol	303	[77]	11	1	18	0.0	2.0
134	1,1,2,2-Tetrabromoethane	1-Hexanol	293	[77]	11	2	19	0.2	2.1
135	1,1,2,2-Tetrabromoethane	1-Hexanol	303	[77]	11	1	14	0.1	1.6
136	1,1,2,2-Tetrabromoethane	1-Octanol	293	[77]	11	1	28	0.1	3.3
137	1,1,2,2-Tetrabromoethane	1-Octanol	303	[77]	11	2	24	0.1	2.7
138	1,1,2,2-Tetrabromoethane	1-Pentanol	293	[77]	11	4	16	0.4	1.8
139	1,1,2,2-Tetrabromoethane	1-Pentanol	303	[77]	11	2	13	0.2	1.5
140	1,3-Dioxolane	1-Chlorobutane	298	[29]	13	3	16	0.3	1.5
141	1,3-Dioxolane	1-Chlorobutane	313	[29]	13	3	4	0.3	0.4
142	1,3-Dioxolane	2-Chlorobutane	298	[29]	13	2	12	0.2	1.2
143	1,3-Dioxolane	2-Chlorobutane	313	[29]	13	3	3	0.3	0.2
144	1,3-Dioxolane	2-Methyl-2-chloropropane	298	[29]	13	2	8	0.2	0.8

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Table 2 (*continued*)

No.	Solvent 1	Solvent 2	T/K	Ref	N	MRD Eq. (6)	MRD Eq. (7)	d_{rms} Eq. (6)	d_{rms} Eq. (7)
145	1,3-Dioxolane	2-Methyl-2-chloropropane	313	[29]	13	1	9	0.1	0.9
146	1,3-Dioxolane	2,2,4-Trimethylpentane	288	[30]	21	9	21	0.8	1.9
147	1,3-Dioxolane	2,2,4-Trimethylpentane	298	[30]	21	7	10	0.7	0.9
148	1,3-Dioxolane	2,2,4-Trimethylpentane	308	[30]	21	7	2	0.6	0.2
149	1,4-Dioxane	1-Chlorobutane	298	[29]	13	7	20	0.7	2.4
150	1,4-Dioxane	1-Chlorobutane	313	[29]	13	6	23	0.6	2.9
151	1,4-Dioxane	2-Chlorobutane	298	[29]	13	6	22	0.5	2.7
152	1,4-Dioxane	2-Chlorobutane	313	[29]	13	5	26	0.5	3.3
153	1,4-Dioxane	2-Methyl-2-chloropropane	298	[29]	13	4	31	0.3	3.8
154	1,4-Dioxane	2-Methyl-2-chloropropane	313	[29]	13	3	33	0.3	4.2
155	1,4-Dioxane	Benzene	298	[31]	7	1	24	0.1	2.9
156	1,4-Dioxane	Ethanol	298	[32]	7	3	22	0.3	2.6
157	1,4-Dioxane	Ethenylbenzene	298	[10]	11	5	31	0.5	3.9
158	1,4-Dioxane	Ethenylbenzene	303	[10]	11	5	32	0.6	4.1
159	1,4-Dioxane	Ethenylbenzene	308	[10]	11	5	33	0.5	4.2
160	1,4-Dioxane	Methanol	298	[32]	7	5	27	0.5	3.3
161	1,4-Dioxane	Tetrachloromethane	298	[31]	7	4	42	0.5	5.4
162	1,8-Cineole	Hexane	298	[8]	13	11	34	1.0	3.7
163	2-(2-Methoxyethoxy)ethanol	Ethyl tert-butyl ether	293	[33]	21	2	13	0.2	1.2
164	2-(2-Methoxyethoxy)ethanol	Ethyl tert-butyl ether	298	[33]	21	2	8	0.2	0.8
165	2-(2-Methoxyethoxy)ethanol	Ethyl tert-butyl ether	303	[33]	21	2	6	0.2	0.6
166	2-[2-(2-Methoxyethoxy)ethoxy]ethanol	Ethyl tert-butyl ether	293	[33]	21	4	18	0.4	1.6
167	2-[2-(2-Methoxyethoxy)ethoxy]ethanol	Ethyl tert-butyl ether	298	[33]	21	3	16	0.3	1.5
168	2-[2-(2-Methoxyethoxy)ethoxy]ethanol	Ethyl tert-butyl ether	303	[33]	21	4	14	0.4	1.3
169	2-Butanol	2-Butanone	293	[34]	16	19	31	1.7	2.6
170	2-Butanol	2-Butanone	298	[34]	16	8	38	0.7	3.1
171	2-Butanol	2-Butanone	303	[34]	16	15	47	1.4	3.6
172	2-Butanol	2-Butanone	308	[34]	16	21	52	1.8	4.0
173	2-Butanol	2-Butanone	313	[34]	16	10	36	0.9	2.9
174	2-Butanol	Anisole	303	[35]	11	15	12	1.3	1.2
175	2-Butanol	Anisole	313	[35]	11	11	13	1.0	1.3
176	2-Butanol	Anisole	323	[35]	11	6	14	0.6	1.4
177	2-Butanol	Decane	293	[36]	13	27	14	2.3	1.4
178	2-Butanol	Decane	298	[36]	13	25	14	2.2	1.4
179	2-Butanol	Decane	303	[36]	13	23	14	2.0	1.4
180	2-Butanol	Dodecane	293	[36]	13	27	20	2.3	2.3
181	2-Butanol	Dodecane	298	[36]	13	25	20	2.1	2.3
182	2-Butanol	Dodecane	303	[36]	13	23	21	1.9	2.4
183	2-Butanol	Methylcyclohexane	298	[37]	15	13	7	1.2	0.7
184	2-Butanol	Octane	293	[36]	13	27	26	2.3	2.3
185	2-Butanol	Octane	298	[36]	13	25	25	2.1	2.2
186	2-Butanol	Octane	303	[36]	13	22	24	1.9	2.1
187	2-Butanol	Propylene glycol monoethyl ether	298	[19]	26	4	21	0.4	2.4
188	2-Butanol	Propylene glycol monomethyl ether	298	[19]	25	3	15	0.3	1.6
189	2-Butanol	Propylene glycol monopropyl ether	298	[19]	24	8	32	0.9	3.9
190	2-Chloroethanol	1-Butanol	298	[10]	11	2	18	0.2	2.0
191	2-Chloroethanol	1-Butanol	303	[10]	11	2	17	0.2	1.8
192	2-Chloroethanol	1-Butanol	308	[10]	11	2	15	0.2	1.7
193	2-Chloroethanol	1-Propanol	298	[10]	11	2	10	0.1	1.1
194	2-Chloroethanol	1-Propanol	303	[10]	11	1	11	0.1	1.1
195	2-Chloroethanol	1-Propanol	308	[10]	11	1	9	0.1	1.0
196	2-Chloroethanol	Butyl acetate	298	[25]	11	1	4	0.1	0.4
197	2-Chloroethanol	Butyl acetate	303	[25]	11	2	4	0.2	0.4
198	2-Chloroethanol	Butyl acetate	308	[25]	11	3	4	0.3	0.4
199	2-Chloroethanol	Ethanol	298	[10]	11	1	10	0.1	1.1
200	2-Chloroethanol	Ethanol	303	[10]	11	1	10	0.1	1.0
201	2-Chloroethanol	Ethanol	308	[10]	11	2	10	0.2	1.0
202	2-Chloroethanol	Ethyl acetate	298	[25]	11	1	5	0.1	0.5
203	2-Chloroethanol	Ethyl acetate	303	[25]	11	2	4	0.2	0.4
204	2-Chloroethanol	Ethyl acetate	308	[25]	11	3	3	0.3	0.3
205	2-Chloroethanol	Methanol	298	[10]	11	9	18	0.9	2.0
206	2-Chloroethanol	Methanol	303	[10]	11	9	18	1.0	2.0
207	2-Chloroethanol	Methanol	308	[10]	11	9	18	1.0	2.0
208	2-Chloroethanol	Methyl acetate	298	[25]	11	3	8	0.3	0.8
209	2-Chloroethanol	Methyl acetate	303	[25]	11	3	9	0.3	1.0
210	2-Chloroethanol	Methyl acetate	308	[25]	11	4	11	0.4	1.1
211	2-Chloroethanol	Propyl acetate	298	[25]	11	2	4	0.2	0.4
212	2-Chloroethanol	Propyl acetate	303	[25]	11	2	3	0.2	0.3
213	2-Chloroethanol	Propyl acetate	308	[25]	11	3	4	0.3	0.4
214	2-Heptanol	Methylcyclohexane	298	[37]	15	4	8	0.4	0.8
215	2-Heptanol	Toluene	298	[38]	21	8	35	0.8	2.9
216	2-Heptanol	Toluene	308	[38]	21	4	29	0.4	2.5
217	2-Hexanol	Methylcyclohexane	298	[37]	15	8	11	0.8	1.1

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Table 2 (*continued*)

No.	Solvent 1	Solvent 2	T/K	Ref	N	MRD Eq. (6)	MRD Eq. (7)	d_{rms} Eq. (6)	d_{rms} Eq. (7)
218	2-Hexanol	Toluene	298	[38]	21	3	26	0.3	2.3
219	2-Hexanol	Toluene	308	[38]	21	9	35	0.8	3.0
220	2-Methoxyethanol	Ethyl tert-butyl ether	293	[33]	21	2	22	0.2	2.0
221	2-Methoxyethanol	Ethyl tert-butyl ether	298	[33]	21	2	19	0.2	1.7
222	2-Methoxyethanol	Ethyl tert-butyl ether	303	[33]	21	2	16	0.2	1.4
223	2-Methyl-1-propanol	2-Butanone	293	[34]	15	24	30	2.1	2.6
224	2-Methyl-1-propanol	2-Butanone	298	[34]	17	14	35	1.2	3.0
225	2-Methyl-1-propanol	2-Butanone	303	[34]	16	16	41	1.4	3.3
226	2-Methyl-1-propanol	2-Butanone	308	[34]	16	13	36	1.2	3.0
227	2-Methyl-1-propanol	2-Butanone	313	[34]	16	16	40	1.4	3.2
228	2-Methyl-1-propanol	Anisole	303	[35]	11	22	14	1.9	1.4
229	2-Methyl-1-propanol	Anisole	313	[35]	11	19	14	1.7	1.4
230	2-Methyl-1-propanol	Anisole	323	[35]	11	16	15	1.4	1.5
231	2-Methyl-1-propanol	Methylcyclohexane	298	[18]	11	3	15	0.3	1.7
232	2-Methyl-1-propanol	Methylcyclohexane	303	[18]	11	3	15	0.3	1.6
233	2-Methyl-1-propanol	Methylcyclohexane	308	[18]	11	3	14	0.3	1.5
234	2-Methyl-1-propanol	Trichloroethylene	293	[39]	8	23	15	2.8	1.7
235	2-Methyl-1-propanol	Trichloroethylene	303	[39]	8	20	14	2.4	1.5
236	2-Methyl-1-propanol	Trichloroethylene	313	[39]	8	18	13	2.1	1.4
237	2-Methyl-2-butanol	2-Butanone	293	[34]	16	28	39	2.3	3.2
238	2-Methyl-2-butanol	2-Butanone	298	[34]	16	11	37	1.0	3.1
239	2-Methyl-2-butanol	2-Butanone	303	[34]	16	18	31	1.6	2.7
240	2-Methyl-2-butanol	2-Butanone	308	[34]	16	12	25	1.2	2.3
241	2-Methyl-2-butanol	2-Butanone	313	[34]	16	18	40	1.6	3.3
242	2-Methyl-2-propanol	Anisole	303	[35]	11	20	12	1.7	1.3
243	2-Methyl-2-propanol	Anisole	313	[35]	11	10	10	0.9	1.1
244	2-Methyl-2-propanol	Anisole	323	[35]	11	3	10	0.3	1.1
245	2-Methyl-2-propanol	Toluene	298	[20]	11	38	35	3.0	3.2
246	2-Methyl-2-propanol	Toluene	303	[20]	11	32	32	2.7	2.9
247	2-Methyl-2-propanol	Toluene	308	[20]	11	28	30	2.4	2.6
248	2-Methyl-2-propanol	Toluene	313	[20]	11	25	31	2.2	2.7
249	2-Methyl-2-propanol	Toluene	318	[20]	11	21	29	1.9	2.5
250	2-Octanol	Cyclohexane	303	[15]	12	8	23	0.9	2.7
251	2-Octanol	Methylcyclohexane	298	[37]	18	2	8	0.2	0.8
252	2-Octanol	Toluene	298	[38]	21	8	33	0.7	2.8
253	2-Octanol	Toluene	308	[38]	21	7	33	0.6	2.9
254	2-Pentanol	Cyclohexane	303	[15]	11	3	20	0.3	2.3
255	2-Pentanol	Methylcyclohexane	298	[37]	16	13	11	1.2	1.1
256	2-Propanol	1,3-Dioxolane	288	[30]	21	24	17	2.1	2.1
257	2-Propanol	1,3-Dioxolane	298	[30]	21	19	19	1.7	2.3
258	2-Propanol	1,3-Dioxolane	308	[30]	21	16	20	1.4	2.5
259	2-Propanol	2-Butanone	293	[34]	16	6	18	0.6	1.6
260	2-Propanol	2-Butanone	298	[34]	16	3	26	0.3	2.2
261	2-Propanol	2-Butanone	303	[34]	16	3	24	0.3	2.0
262	2-Propanol	2-Butanone	308	[34]	16	2	23	0.2	2.0
263	2-Propanol	2-Butanone	313	[34]	16	2	22	0.2	1.9
264	2-Propanol	Anisole	298	[11]	11	16	8	1.4	0.8
265	2-Propanol	Anisole	303	[11]	11	14	8	1.3	0.8
266	2-Propanol	Anisole	308	[11]	11	13	8	1.2	0.8
267	2-Propanol	Cyclohexane	303	[15]	11	3	21	0.3	2.5
268	2-Propanol	Mesitylene	298	[17]	11	16	30	1.4	2.6
269	2-Propanol	Mesitylene	303	[17]	11	15	29	1.3	2.5
270	2-Propanol	Mesitylene	308	[17]	11	14	27	1.3	2.3
271	2-Propanol	Methylcyclohexane	298	[37]	17	12	5	1.1	0.5
272	2-Propanol	Methylcyclohexane	298	[18]	11	10	7	0.9	0.7
273	2-Propanol	Methylcyclohexane	303	[18]	11	8	7	0.8	0.7
274	2-Propanol	Methylcyclohexane	308	[18]	11	8	7	0.7	0.7
275	2-Propanol	Tetrahydrofuran	293	[28]	11	3	4	0.3	0.4
276	2-Propanol	Tetrahydrofuran	303	[28]	11	10	15	0.9	1.4
277	2-Propanol	Tetrahydrofuran	313	[28]	11	7	15	0.7	1.5
278	2-Propanol	Trichloroethylene	293	[39]	8	17	10	1.9	0.9
279	2-Propanol	Trichloroethylene	303	[39]	8	15	9	1.7	0.9
280	2-Propanol	Trichloroethylene	313	[39]	8	13	9	1.5	0.8
281	3-Methyl-1-butanol	Anisole	298	[11]	11	15	9	1.4	1.0
282	3-Methyl-1-butanol	Anisole	303	[11]	11	14	10	1.3	1.0
283	3-Methyl-1-butanol	Anisole	308	[11]	11	7	38	0.6	3.1
284	3-Methyl-1-butanol	Mesitylene	298	[17]	11	15	29	1.3	2.5
285	3-Methyl-1-butanol	Mesitylene	303	[17]	11	13	27	1.2	2.4
286	3-Methyl-1-butanol	Mesitylene	308	[17]	11	12	26	1.2	2.3
287	3-Methyl-1-butanol	Methylcyclohexane	298	[18]	11	22	26	2.6	3.0
288	3-Methyl-1-butanol	Methylcyclohexane	303	[18]	11	21	25	2.5	2.8
289	3-Methyl-1-butanol	Methylcyclohexane	308	[18]	11	18	23	2.1	2.5

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Table 2 (*continued*)

No.	Solvent 1	Solvent 2	T/K	Ref	N	MRD Eq. (6)	MRD Eq. (7)	d_{rms} Eq. (6)	d_{rms} Eq. (7)
290	Acetone	Hexane	298	[40]	7	1	88	0.0	6.2
291	alfa-Pinene	Hexane	298	[8]	13	3	25	0.3	2.3
292	Aniline	Benzene	298	[41]	11	2	22	0.2	2.0
293	Aniline	Benzene	303	[41]	11	2	20	0.2	1.8
294	Aniline	Benzene	308	[41]	11	3	19	0.3	1.7
295	Aniline	Benzene	313	[41]	11	3	18	0.3	1.6
296	Anisole	Decane	293	[42]	11	10	11	0.9	1.2
297	Anisole	Decane	298	[42]	11	10	10	0.9	1.2
298	Anisole	Decane	303	[42]	11	9	12	0.9	1.3
299	Anisole	Heptane	293	[42]	11	6	22	0.6	2.0
300	Anisole	Heptane	298	[42]	11	6	17	0.6	1.6
301	Anisole	Heptane	303	[42]	11	5	14	0.5	1.3
302	Anisole	Hexane	293	[42]	11	7	41	0.7	3.4
303	Anisole	Hexane	298	[42]	11	8	35	0.7	2.9
304	Anisole	Hexane	303	[42]	11	6	31	0.5	2.6
305	Anisole	Methylcyclohexane	298	[43]	11	5	13	0.5	1.4
306	Anisole	Methylcyclohexane	303	[43]	11	5	15	0.5	1.7
307	Anisole	Methylcyclohexane	308	[43]	11	4	17	0.4	1.9
308	Anisole	Nonane	293	[42]	11	9	7	0.8	0.7
309	Anisole	Nonane	298	[42]	11	9	5	0.9	0.5
310	Anisole	Nonane	303	[42]	11	9	4	0.8	0.5
311	Anisole	Octane	293	[42]	11	8	11	0.8	1.1
312	Anisole	Octane	298	[42]	11	8	8	0.8	0.7
313	Anisole	Octane	303	[42]	11	7	5	0.6	0.5
314	Benzene	1-Bromopropane	308	[9]	10	1	12	0.0	1.1
315	Benzene	2,2,4-Trimethylpentane	298	[44]	11	8	45	0.7	3.6
316	Benzene	Acetone	298	[32]	14	2	22	0.2	2.0
317	Benzene	Chloroform	298	[32]	7	3	20	0.3	1.8
318	Benzene	Ethyl acetate	298	[32]	7	3	28	0.3	2.4
319	Benzene	Ethyl ether	298	[32]	7	4	47	0.4	3.9
320	Benzene	Methanol	298	[32]	14	7	21	0.8	1.8
321	Benzene	Tetrahydrofuran	303	[45]	11	4	15	0.4	1.5
322	Benzene	Toluene	298	[32]	7	5	13	0.5	1.2
323	Benzonitrile	Benzene	303	[46]	11	3	6	0.3	0.5
324	Benzonitrile	Ethanol	303	[12]	11	4	24	0.4	2.1
325	Benzonitrile	Ethanol	308	[12]	11	5	21	0.5	1.9
326	Benzonitrile	Methanol	303	[12]	11	13	9	1.4	0.9
327	Benzonitrile	Methanol	308	[12]	11	12	8	1.3	0.8
328	Benzoyl chloride	Benzene	303	[46]	11	10	9	1.1	0.8
329	Benzyl alcohol	Benzene	303	[46]	11	34	26	4.4	2.8
330	beta-Pinene	Hexane	298	[8]	14	5	27	0.5	2.7
331	Bromobenzene	Methanol	293	[47]	11	16	9	1.8	0.8
332	Bromobenzene	Methanol	303	[47]	11	13	7	1.5	0.7
333	Bromobenzene	Methanol	313	[47]	11	14	6	1.5	0.6
334	Bromoform	Ethenylbenzene	298	[10]	11	9	18	1.0	2.0
335	Bromoform	Ethenylbenzene	303	[10]	11	9	20	1.0	2.3
336	Bromoform	Ethenylbenzene	308	[10]	11	9	22	0.9	2.6
337	Butyl acetate	Acrylonitrile	298	[10]	11	6	13	0.6	1.4
338	Butyl acetate	Acrylonitrile	303	[10]	11	5	14	0.6	1.5
339	Butyl acetate	Acrylonitrile	308	[10]	11	5	16	0.5	1.8
340	Chlorobenzene	Benzene	303	[46]	11	4	9	0.4	0.8
341	Chlorobenzene	Methanol	293	[47]	11	15	11	1.6	1.0
342	Chlorobenzene	Methanol	303	[47]	11	12	9	1.4	0.8
343	Chlorobenzene	Methanol	313	[47]	11	12	7	1.3	0.7
344	Chloroform	Acetone	298	[32]	7	10	17	1.1	1.4
345	Chloroform	Methanol	298	[32]	7	11	15	1.2	1.4
346	Chloroform	Methanol	298	[22]	21	13	15	1.5	1.4
347	Chloroform	Methanol	308	[22]	21	12	12	1.4	1.2
348	Chloroform	Methanol	313	[14]	21	12	12	1.3	1.2
349	Cyclohexane	1-Bromobutane	308	[9]	11	3	27	0.3	3.1
350	Cyclohexane	1-Bromopropane	308	[9]	10	3	23	0.3	2.7
351	Cyclohexane	Acetone	298	[40]	7	31	19	2.5	1.8
352	Cyclohexane	Benzene	298	[32]	7	5	17	0.5	1.9
353	Cyclohexane	Bromopentane	308	[9]	11	3	33	0.3	4.0
354	Cyclohexane	Hexane	298	[48]	12	10	26	0.9	2.5
355	Cyclohexane	Tetrachloromethane	298	[32]	7	0	38	0.0	4.8
356	Cyclohexane	Tetrahydrofuran	303	[45]	11	2	30	0.2	3.6
357	Cyclohexane	Toluene	298	[48]	12	9	19	0.8	2.1
358	Cyclohexane	Triethylamine	303	[27]	11	10	24	1.0	2.2
359	Cyclohexanol	Cyclohexane	303	[45]	11	38	82	5.2	19.4
360	di-n-Butylamine	Methanol	303	[49]	10	2	32	0.2	2.6
361	di-n-Butylamine	Methanol	313	[49]	11	2	30	0.1	2.4
362	di-n-Butylamine	Methanol	323	[49]	11	3	27	0.3	2.2

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Table 2 (*continued*)

No.	Solvent 1	Solvent 2	T/K	Ref	N	MRD Eq. (6)	MRD Eq. (7)	d_{rms} Eq. (6)	d_{rms} Eq. (7)
363	Dibutyl ether	Benzene	298	[50]	13	2	11	0.2	1.0
364	Dibutyl ether	Benzene	308	[50]	13	3	3	0.3	0.3
365	Dibutyl ether	p-Xylene	298	[50]	13	2	15	0.2	1.4
366	Dibutyl ether	p-Xylene	308	[50]	13	1	6	0.1	0.5
367	Dibutyl ether	Toluene	298	[50]	13	0	17	0.0	1.6
368	Dibutyl ether	Toluene	308	[50]	13	1	7	0.0	0.6
369	Dimethylformamide	Acetonitrile	298	[32]	7	2	19	0.2	1.7
370	Dimethylformamide	Benzene	298	[51]	7	4	28	0.4	2.4
371	Dimethylformamide	Ethenylbenzene	298	[10]	11	8	14	0.8	1.2
372	Dimethylformamide	Ethenylbenzene	303	[10]	11	8	11	0.8	1.0
373	Dimethylformamide	Ethenylbenzene	308	[10]	11	7	9	0.8	0.9
374	Dimethylformamide	Methanol	298	[52]	7	11	16	1.2	1.5
375	Dimethylformamide	Toluene	278	[53]	12	1	62	0.1	4.7
376	Dimethylformamide	Toluene	283	[53]	12	1	53	0.1	4.2
377	Dimethylformamide	Toluene	293	[53]	12	1	36	0.1	3.0
378	Dimethysulfoxide	Acetone	298	[54]	7	5	13	0.5	1.4
379	Dimethysulfoxide	Acetonitrile	298	[55]	7	2	11	0.2	1.1
380	Dimethysulfoxide	Benzene	298	[56]	11	2	4	0.2	0.4
381	Dimethysulfoxide	Benzene	298	[57]	7	13	18	1.5	2.0
382	Dimethysulfoxide	Benzene	303	[56]	11	2	4	0.2	0.4
383	Dimethysulfoxide	Benzene	308	[56]	11	2	6	0.2	0.6
384	Dimethysulfoxide	Benzene	313	[56]	11	1	8	0.1	0.9
385	Dimethysulfoxide	Benzene	318	[56]	11	0	11	0.0	1.2
386	Dimethysulfoxide	Ethanol	298	[58]	7	4	13	0.4	1.3
387	Dimethysulfoxide	Ethenylbenzene	298	[10]	11	2	5	0.2	0.5
388	Dimethysulfoxide	Ethenylbenzene	303	[10]	11	3	6	0.3	0.6
389	Dimethysulfoxide	Ethenylbenzene	308	[10]	11	3	7	0.3	0.7
390	Dimethysulfoxide	m-Xylene	298	[56]	11	7	16	0.7	1.5
391	Dimethysulfoxide	m-Xylene	303	[56]	11	7	14	0.6	1.3
392	Dimethysulfoxide	m-Xylene	308	[56]	11	7	13	0.7	1.2
393	Dimethysulfoxide	m-Xylene	313	[56]	11	7	11	0.7	1.1
394	Dimethysulfoxide	m-Xylene	318	[56]	11	7	9	0.7	1.0
395	Dimethysulfoxide	Mesitylene	298	[56]	11	3	8	0.3	0.8
396	Dimethysulfoxide	Mesitylene	303	[56]	11	4	7	0.4	0.7
397	Dimethysulfoxide	Mesitylene	308	[56]	11	4	7	0.4	0.7
398	Dimethysulfoxide	Mesitylene	313	[56]	11	4	7	0.4	0.7
399	Dimethysulfoxide	Mesitylene	318	[56]	11	4	9	0.4	0.9
400	Dimethysulfoxide	Methanol	298	[58]	7	12	12	1.4	1.3
401	Dimethysulfoxide	Nitromethane	298	[59]	7	7	20	0.7	2.3
402	Dimethysulfoxide	o-Xylene	298	[56]	11	7	5	0.6	0.5
403	Dimethysulfoxide	o-Xylene	303	[56]	11	8	6	0.7	0.6
404	Dimethysulfoxide	o-Xylene	308	[56]	11	9	6	0.8	0.7
405	Dimethysulfoxide	o-Xylene	313	[56]	11	9	8	0.8	0.8
406	Dimethysulfoxide	o-Xylene	318	[56]	11	9	10	0.8	1.1
407	Dimethysulfoxide	p-Xylene	298	[56]	11	6	13	0.6	1.2
408	Dimethysulfoxide	p-Xylene	303	[56]	11	8	12	0.7	1.2
409	Dimethysulfoxide	p-Xylene	308	[56]	11	8	10	0.8	1.0
410	Dimethysulfoxide	p-Xylene	313	[56]	11	9	9	0.8	1.0
411	Dimethysulfoxide	p-Xylene	318	[56]	11	9	8	0.8	0.8
412	Dimethysulfoxide	Tetrachloromethane	298	[59]	7	4	19	0.4	1.9
413	Dimethysulfoxide	Toluene	298	[56]	11	2	11	0.2	1.0
414	Dimethysulfoxide	Toluene	303	[56]	11	2	9	0.2	0.9
415	Dimethysulfoxide	Toluene	308	[56]	11	3	7	0.3	0.8
416	Dimethysulfoxide	Toluene	313	[56]	11	3	8	0.2	0.8
417	Dimethysulfoxide	Toluene	318	[56]	11	2	8	0.2	0.9
418	Dodecane	Anisole	293	[42]	11	12	15	1.1	1.4
419	Dodecane	Anisole	298	[42]	11	13	12	1.2	1.2
420	Dodecane	Anisole	303	[42]	11	12	11	1.1	1.1
421	Ethanol	Acetone	298	[32]	14	5	7	0.5	0.6
422	Ethanol	Acetonitrile	298	[60]	14	12	13	1.1	1.2
423	Ethanol	Acrylonitrile	298	[25]	11	4	12	0.4	1.1
424	Ethanol	Acrylonitrile	303	[25]	11	5	9	0.4	0.8
425	Ethanol	Acrylonitrile	308	[25]	11	3	6	0.3	0.6
426	Ethanol	Anisole	298	[11]	11	2	9	0.1	0.9
427	Ethanol	Anisole	303	[11]	11	2	9	0.2	1.0
428	Ethanol	Anisole	308	[11]	11	2	10	0.2	1.0
429	Ethanol	Benzene	298	[32]	14	3	13	0.3	1.2
430	Ethanol	Chloroform	298	[32]	7	4	5	0.4	0.5
431	Ethanol	Chloroform	313	[14]	21	3	5	0.4	0.5
432	Ethanol	Cyclohexane	298	[40]	7	10	27	1.0	3.4
433	Ethanol	Cyclohexane	303	[15]	11	2	21	0.2	2.5
434	Ethanol	Dimethoxyethane	298	[16]	11	6	12	0.6	1.1

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Table 2 (*continued*)

No.	Solvent 1	Solvent 2	T/K	Ref	N	MRD Eq. (6)	MRD Eq. (7)	d_{rms} Eq. (6)	d_{rms} Eq. (7)
435	Ethanol	Dimethylformamide	298	[61]	7	4	23	0.4	2.9
436	Ethanol	Ethyl acetate	298	[62]	7	5	10	0.4	0.9
437	Ethanol	Ethyl ether	298	[32]	7	16	21	1.8	1.8
438	Ethanol	Hexane	298	[40]	7	17	18	1.9	1.5
439	Ethanol	Mesitylene	298	[17]	11	2	18	0.2	1.6
440	Ethanol	Mesitylene	303	[17]	11	1	18	0.1	1.6
441	Ethanol	Mesitylene	308	[17]	11	1	15	0.1	1.4
442	Ethanol	Methanol	298	[32]	14	4	12	0.4	1.3
443	Ethanol	Methylcyclohexane	298	[37]	16	3	10	0.3	1.0
444	Ethanol	Methylcyclohexane	298	[18]	11	2	11	0.2	1.2
445	Ethanol	Methylcyclohexane	303	[18]	11	3	12	0.3	1.3
446	Ethanol	Methylcyclohexane	308	[18]	11	2	12	0.2	1.3
447	Ethanol	Nitromethane	298	[63]	14	4	18	0.4	2.2
448	Ethanol	Pyridine	298	[32]	7	7	24	0.8	2.9
449	Ethanol	Tetrachloromethane	298	[32]	14	8	18	0.8	2.1
450	Ethanol	Toluene	298	[32]	7	7	9	0.7	0.8
451	Ethanol	Trichloroethane	293	[39]	8	11	10	1.2	0.9
452	Ethanol	Trichloroethane	303	[39]	8	11	8	1.2	0.8
453	Ethanol	Trichloroethane	313	[39]	8	11	9	1.1	0.9
454	Ethanol	Trichloromethane	298	[22]	21	4	7	0.4	0.7
455	Ethanol	Trichloromethane	308	[22]	21	4	4	0.4	0.4
456	Ethenylbenzene	Chloroform	298	[10]	11	8	19	0.8	1.6
457	Ethenylbenzene	Chloroform	303	[10]	11	8	13	0.9	1.2
458	Ethenylbenzene	Chloroform	308	[10]	11	8	9	0.8	0.8
459	Ethenylbenzene	Tetrahydrofuran	298	[10]	11	10	18	1.1	1.7
460	Ethenylbenzene	Tetrahydrofuran	303	[10]	11	10	18	1.1	1.8
461	Ethenylbenzene	Tetrahydrofuran	308	[10]	11	10	19	1.0	1.9
462	Ethyl acetate	Acetonitrile	298	[64]	7	13	19	1.5	2.0
463	Ethyl acetate	Acrylonitrile	298	[10]	11	4	8	0.4	0.7
464	Ethyl acetate	Acrylonitrile	303	[10]	11	4	8	0.4	0.7
465	Ethyl acetate	Acrylonitrile	308	[10]	11	3	8	0.3	0.9
466	Ethylene glycol	Methyl acetate	298	[10]	11	14	18	1.5	2.1
467	Ethylene glycol	Methyl acetate	303	[10]	11	10	13	1.1	1.5
468	Ethylene glycol	Methyl acetate	308	[10]	11	10	12	1.0	1.4
469	Formamide	1-Propanol	293	[65]	13	8	12	0.9	1.0
470	Formamide	1-Propanol	298	[65]	13	9	10	1.0	0.9
471	Formamide	1-Propanol	303	[65]	13	10	9	1.1	0.8
472	Formamide	1-Propanol	308	[65]	13	11	9	1.2	0.9
473	Formamide	1-Propanol	313	[65]	13	12	9	1.4	0.8
474	Formamide	1-Propanol	318	[65]	13	13	9	1.5	0.9
475	Formamide	Ethanol	293	[65]	13	6	21	0.7	1.8
476	Formamide	Ethanol	298	[65]	13	6	17	0.7	1.5
477	Formamide	Ethanol	303	[65]	13	6	16	0.7	1.4
478	Formamide	Ethanol	308	[65]	13	6	15	0.6	1.4
479	Formamide	Ethanol	313	[65]	13	6	13	0.6	1.2
480	Formamide	Ethanol	318	[65]	13	6	10	0.7	1.0
481	Glycerol	Ethanol	294	[66]	20	26	40	3.1	5.7
482	m-Cresol	o-Cresol	313	[67]	11	2	35	0.2	2.7
483	m-Cresol	o-Cresol	323	[8]	11	1	58	0.1	4.3
484	m-Cresol	o-Cresol	333	[67]	11	1	68	0.1	5.0
485	m-Xylene	2,2,4-Trimethylpentane	298	[44]	10	1	58	0.1	4.5
486	Methanol	Acetone	298	[32]	14	9	5	0.9	0.5
487	Methanol	Acetonitrile	298	[55]	14	2	2	0.2	0.2
488	Methanol	Acrylonitrile	298	[25]	11	4	3	0.4	0.3
489	Methanol	Acrylonitrile	303	[25]	11	3	3	0.3	0.3
490	Methanol	Acrylonitrile	308	[25]	11	4	5	0.4	0.5
491	Methanol	Butylamine	303	[49]	11	12	22	1.4	2.0
492	Methanol	Butylamine	313	[49]	11	9	22	0.9	2.0
493	Methanol	Butylamine	323	[49]	11	6	23	0.6	2.1
494	Methanol	Dimethoxyethane	298	[16]	11	5	4	0.6	0.4
495	Methanol	Ethyl acetate	298	[52]	7	5	4	0.5	0.4
496	Methanol	Ethyl ether	298	[32]	7	2	30	0.2	2.5
497	Methanol	tert-Amyl methyl ether	298	[26]	25	9	7	0.9	0.7
498	Methanol	tert-Butyl methyl ether	298	[26]	23	8	7	0.8	0.6
499	Methyl acetate	Acrylonitrile	298	[10]	11	4	14	0.4	1.3
500	Methyl acetate	Acrylonitrile	303	[10]	11	5	11	0.5	1.0
501	Methyl acetate	Acrylonitrile	308	[10]	11	4	9	0.4	0.8
502	Methylcyclohexane	Benzene	298	[43]	11	4	4	0.4	0.4
503	Methylcyclohexane	Benzene	303	[43]	11	6	7	0.6	0.8
504	Methylcyclohexane	Benzene	308	[43]	11	3	5	0.3	0.6
505	Methylcyclohexane	Mesitylene	298	[43]	11	2	5	0.2	0.5
506	Methylcyclohexane	Mesitylene	303	[43]	11	1	4	0.1	0.4
507	Methylcyclohexane	Mesitylene	308	[43]	11	2	5	0.2	0.5

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Table 2 (*continued*)

No.	Solvent 1	Solvent 2	T/K	Ref	N	MRD Eq. (6)	MRD Eq. (7)	d_{rms} Eq. (6)	d_{rms} Eq. (7)
508	Methylcyclohexane	p-Xylene	298	[43]	11	2	7	0.2	0.7
509	Methylcyclohexane	p-Xylene	303	[43]	11	1	6	0.1	0.5
510	Methylcyclohexane	p-Xylene	308	[43]	11	2	5	0.1	0.5
511	Methylcyclohexane	Tetrahydrofuran	303	[45]	11	2	16	0.2	1.8
512	Methylcyclohexane	Toluene	298	[43]	11	2	8	0.2	0.7
513	Methylcyclohexane	Toluene	303	[43]	11	2	7	0.2	0.6
514	Methylcyclohexane	Toluene	308	[43]	11	2	6	0.2	0.6
515	Methylcyclohexane	Trichloroethylene	298	[23]	12	0	5	0.0	0.5
516	Methylcyclopentane	2-Butanone	293	[68]	13	2	20	0.2	1.8
517	Methylcyclopentane	2-Butanone	298	[68]	13	2	15	0.2	1.4
518	Methylcyclopentane	2-Butanone	303	[68]	13	2	11	0.2	1.0
519	Methylcyclopentane	2-Pentanone	293	[68]	13	1	17	0.1	1.6
520	Methylcyclopentane	2-Pentanone	298	[68]	13	1	13	0.1	1.2
521	Methylcyclopentane	2-Pentanone	303	[68]	13	1	9	0.1	0.8
522	Methylcyclopentane	Acetone	293	[68]	13	2	18	0.2	1.6
523	Methylcyclopentane	Acetone	298	[68]	13	3	13	0.3	1.2
524	Methylcyclopentane	Acetone	303	[68]	13	2	9	0.2	0.9
525	N-Methylacetamide	2-Methoxyethanol	308	[69]	22	4	11	0.4	1.2
526	N-Methylacetamide	2-Methoxyethanol	313	[69]	22	4	12	0.4	1.2
527	N-Methylacetamide	2-Methoxyethanol	318	[69]	22	5	12	0.5	1.3
528	N-Methylacetamide	Acetophenone	308	[70]	11	3	17	0.3	1.9
529	N-Methylacetamide	Propiophenone	308	[70]	11	3	10	0.3	1.1
530	N,N-Dimethylacetamide	Ethenylbenzene	298	[10]	11	8	7	0.8	0.7
531	N,N-Dimethylacetamide	Ethenylbenzene	303	[10]	11	8	9	0.8	0.9
532	N,N-Dimethylacetamide	Ethenylbenzene	308	[10]	11	7	11	0.8	1.2
533	Nitrobenzene	Acetone	298	[32]	7	9	8	1.0	0.8
534	Nitrobenzene	Acetonitrile	298	[55]	7	8	12	0.8	1.3
535	Nitrobenzene	Benzene	298	[32]	7	2	7	0.2	0.8
536	Nitrobenzene	Ethanol	298	[71]	7	6	15	0.6	1.4
537	Nitrobenzene	Methanol	298	[71]	7	16	8	1.9	0.8
538	Nitrobenzene	Tetrachloromethane	298	[32]	7	4	23	0.4	2.7
539	Nitromethane	Acetonitrile	298	[72]	14	3	12	0.3	1.2
540	Nitromethane	Benzene	298	[32]	14	3	8	0.3	0.8
541	Nitromethane	Ethyl acetate	298	[73]	7	2	9	0.2	0.9
542	Nitromethane	Methanol	298	[63]	14	2	15	0.2	1.4
543	o-Xylene	2,2,4-Trimethylpentane	298	[44]	11	2	31	0.2	2.7
544	p-Cresol	m-Cresol	313	[67]	11	5	31	0.6	2.9
545	p-Cresol	m-Cresol	323	[67]	11	6	32	0.6	2.5
546	p-Cresol	m-Cresol	333	[67]	11	6	36	0.6	2.7
547	p-Cresol	o-Cresol	313	[67]	11	1	30	0.1	2.4
548	p-Cresol	o-Cresol	323	[67]	11	2	51	0.1	3.9
549	p-Cresol	o-Cresol	333	[67]	11	1	62	0.1	4.6
550	p-Cymene	Hexane	298	[8]	14	6	59	0.9	4.9
551	p-Xylene	2,2,4-Trimethylpentane	298	[44]	11	2	53	0.2	4.1
552		Tetrahydrofuran	303	[45]	11	5	20	0.5	1.8
553	Propyl acetate	Acrylonitrile	298	[10]	11	4	9	0.4	1.0
554	Propyl acetate	Acrylonitrile	303	[10]	11	5	11	0.5	1.2
555	Propyl acetate	Acrylonitrile	308	[10]	11	5	13	0.5	1.4
556	Propylbenzene	Tetrahydrofuran	303	[45]	11	6	18	0.6	1.8
557	Propylene glycol tert-butyl ether	1-Butanol	298	[19]	26	14	31	1.5	3.9
558	Propylene glycol tert-butyl ether	2-Butanol	298	[19]	25	7	33	0.7	4.1
559	Pyridine	Acetonitrile	298	[32]	7	8	15	0.8	1.6
560	Pyridine	Benzene	298	[32]	7	4	8	0.4	0.9
561	Pyridine	Methanol	298	[52]	7	13	7	1.4	0.7
562	tert-Butanol	Butylamine	293	[13]	11	36	26	2.9	2.8
563	tert-Butanol	Butylamine	303	[13]	11	23	23	1.9	2.7
564	tert-Butanol	Butylamine	313	[13]	11	13	35	1.2	4.5
565	Tetrachloromethane	Acetone	298	[32]	7	5	15	0.5	1.7
566	Tetrachloromethane	Acetonitrile	298	[74]	7	3	19	0.3	2.1
567	Tetrachloromethane	Benzene	298	[32]	7	2	16	0.2	1.7
568	Tetrachloromethane	Chloroform	298	[32]	7	1	12	0.1	1.3
569	Tetrachloromethane	Dimethylformamide	298	[59]	7	4	19	0.3	2.2
570	Tetrachloromethane	Ethyl acetate	298	[59]	7	9	5	0.8	0.5
571	Tetrachloromethane	Methanol	298	[32]	7	16	17	1.8	1.9
572	Tetrachloromethane	Nitromethane	298	[32]	7	1	37	0.1	4.8
573	Tetrachloromethane	Nitromethane	298	[59]	7	7	26	0.7	3.1
574	Tetrahydrofuran	Hexane	303	[45]	11	2	23	0.2	2.0
575	Toluene	2,2,4-Trimethylpentane	298	[44]	11	3	51	0.3	4.0
576	Toluene	Acetonitrile	298	[75]	7	4	20	0.4	1.7
577	Toluene	Hexane	298	[48]	12	6	64	0.6	5.0
578	Toluene	Methanol	298	[76]	7	11	28	1.1	2.3
579	Toluene	Tetrahydrofuran	303	[45]	11	5	18	0.5	1.7
580	tri-n-Butylamine	Cyclohexane	303	[27]	11	13	27	1.2	3.2
			Overall			7	17	0.7	1.7

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relationship between viscosity, temperature and Abraham parameters of the mono-solvents, and Eq. (3) can be written as

$$\begin{aligned}\log \eta_{m,T} = {} & x_1\gamma_1 + \frac{x_1}{T}\left\{\alpha_0 + \alpha_1 E_1 + \alpha_2 S_1 + \alpha_3 A_1 + \alpha_4 B_1 + \alpha_5 V_1\right.\\ & \left. + \alpha_6 A_1\cdot B_1 + \alpha_7\frac{A_1}{V_1} + \alpha_8\frac{B_1}{V_1} + \alpha_9\frac{A_1\cdot B_1}{V_1}\right\} + x_2\gamma_2\\ & + \frac{x_2}{T}\left\{\beta_0 + \beta_1 E_2 + \beta_2 S_2 + \beta_3 A_2 + \beta_4 B_2 + \beta_5 V_2\right.\\ & \left. + \beta_6 A_2\cdot B_2 + \beta_7\frac{A_2}{V_2} + \beta_8\frac{B_2}{V_2} + \beta_9\frac{A_2\cdot B_2}{V_2}\right\}\\ & + \frac{x_1x_2}{T}\left[W_0 + W_1(E_1-E_2)^2 + W_2(S_1-S_2)^2\right.\\ & \left. + W_3(A_1-A_2)^2 + W_4(B_1-B_2)^2 + W_5(V_1-V_2)^2\right]\\ & + \frac{x_1x_2(x_1-x_2)}{T}\left[W_0' + W_1'(E_1-E_2)^2 + W_2'(S_1-S_2)^2\right.\\ & \left. + W_3'(A_1-A_2)^2 + W_4'(B_1-B_2)^2 + W_5'(V_1-V_2)^2\right]\\ & + \frac{x_1x_2(x_1-x_2)^2}{T}\left[W_0'' + W_1''(E_1-E_2)^2 + W_2''(S_1-S_2)^2\right.\\ & \left. + W_3''(A_1-A_2)^2 + W_4''(B_1-B_2)^2 + W_5''(V_1-V_2)^2\right]\end{aligned} \quad (4)$$

where γ_1, γ_2, α, β and W terms are the model constants. The numerical values of these terms could be computed by regression $\log \eta_{\eta,T}$ against

$x_1, \frac{x_1}{T}, \frac{x_1E_1}{T}, \frac{x_1S_1}{T}, \frac{x_1A_1}{T}, \frac{x_1B_1}{T}, \frac{x_1V_1}{T}, \frac{x_1A_1\cdot B_1}{T}, \frac{x_1A_1}{T\cdot V_1}, \frac{x_1B_1}{T\cdot V_1}, \frac{x_1A_1\cdot B_1}{T\cdot V_1}, x_2, \frac{x_2}{T}, \frac{x_2E_2}{T}$,
$\frac{x_2S_2}{T}, \frac{x_2A_2}{T}, \frac{x_2B_2}{T}, \frac{x_2V_2}{T}, \frac{x_2A_2\cdot B_2}{T}, \frac{x_2A_2}{T\cdot V_2}, \frac{x_2B_2}{T\cdot V_2}, \frac{x_2A_2\cdot B_2}{T\cdot V_2}, \frac{x_1x_2}{T}, \frac{x_1x_2(E_1-E_2)^2}{T}$,
$\frac{x_1x_2(S_1-S_2)^2}{T}, \frac{x_1x_2(A_1-A_2)^2}{T}, \frac{x_1x_2(B_1-B_2)^2}{T}, \frac{x_1x_2(V_1-V_2)^2}{T}$,
$\frac{x_1x_2(x_1-x_2)}{T}, \frac{x_1x_2(x_1-x_2)(E_1-E_2)^2}{T}, \frac{x_1x_2(x_1-x_2)(S_1-S_2)^2}{T}$,
$\frac{x_1x_2(x_1-x_2)(A_1-A_2)^2}{T}, \frac{x_1x_2(x_1-x_2)(B_1-B_2)^2}{T}, \frac{x_1x_2(x_1-x_2)(V_1-V_2)^2}{T}$,
$\frac{x_1x_2(x_1-x_2)^2}{T}, \frac{x_1x_2(x_1-x_2)^2(E_1-E_2)^2}{T}, \frac{x_1x_2(x_1-x_2)^2(S_1-S_2)^2}{T}$,
$\frac{x_1x_2(x_1-x_2)^2(A_1-A_2)^2}{T}, \frac{x_1x_2(x_1-x_2)^2(B_1-B_2)^2}{T}$

and $\frac{x_1x_2(x_1-x_2)^2(V_1-V_2)^2}{T}$. The W terms represent the contribution of different types of interactions in the two-body and three-body interaction terms of the original model.

2.2. Experimental data

The details of the collected data sets from the literature [8–77], are given in Table 2. These data sets include non-aqueous binary mixtures at various temperatures. In all computations, solvents 1 and 2 are defined by condition of $\eta_1 > \eta_2$.

The fitness of the experimental data to the model was studied by calculating the correlation coefficient and the accuracy criteria. The validity of the proposed model was assessed using cross-validation methods: The model constants calculated using odd set numbers was used to predict the viscosity of even set numbers and vice versa.

The accuracy of the viscosity was investigated by computing the mean relative deviation (MRD) using

$$MRD = \frac{100}{N}\sum\left(\frac{\left|\eta^{Calc} - \eta^{Exp}\right|}{\eta^{Exp}}\right) \quad (5)$$

in which N is the number of data points. The individual relative deviations $IRD = \frac{100\cdot\left|\eta^{Calc} - \eta^{Exp}\right|}{\eta^{Exp}}$ are also computed to present the error of each data point. The IRDs are sorted in 5 subgroups, i.e. IRD ≤ 5, IRD of 5–10, 10–15, 15–20 and IRDs > 20%.

3. Results and discussion

3.1. Modeling viscosity using mono-solvent data

Available viscosity data of binary solvent mixtures at various temperatures were fitted to Eq. (3) and the obtained model was

$$\begin{aligned}\ln \eta_{m,T} = {} & x_1 \ln \eta_{1,T} + x_2 \ln \eta_{2,T}\\ & + \frac{x_1x_2}{T}\left[-61.784 + 54.566(E_1-E_2)^2 - 129.759(S_1-S_2)^2 - 1978.988(A_1-A_2)^2\right.\\ & \left. + 331.691(B_1-B_2)^2 + 190.370(V_1-V_2)^2\right]\\ & + \frac{x_1x_2(x_1-x_2)}{T}\left[-706.352(A_1-A_2)^2 + 65.119(V_1-V_2)^2\right].\end{aligned} \quad (6)$$

The model was statistically significant with the F value of 578 ($p<0.0005$) and covered the $\eta_{m,T}$ range of 0.226 to 1390. The F value represents the statistical significance of the correlation and is a ratio of mean squares due to regression to mean squares about regression. A correlation is considered significant, when the calculated F value is greater than the critical F value obtained from Fisher distribution with the degrees of freedoms of (number of variables) and (number of observations − number of variables). In Eq. (6), the degrees of freedoms were 8 and 7213, respectively, and the critical F value was 6. When the viscosity data are back-calculated, the resulted MRDs were in the range of around 0 (i.e. <0.5)% (for methylcyclohexane + trichloroethylene at 298 K) and 69% (for 1-hexanol + dimethoxyethane at 298 K) with the overall MRD (±SD) of 7 (±7)%. Details of the MRD values for the investigated systems are listed in Table 2. Fig. 1 shows the relative frequency of IRDs in different subgroups where in ~60% of the cases, the IRD is less than 5%.

To compare the accuracy of Eq. (6) with a similar predictive model from the literature, the results reported by Bertrand [78] were employed. For this purpose, the accuracy criterion of Bertrand (d_{rms})

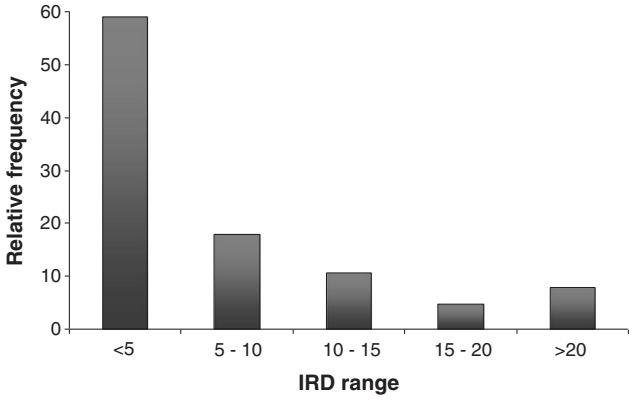

Fig. 1. The relative frequency of individual relative deviations (IRD) for predicted viscosity of binary mixtures using Eq. (6) employing two experimental viscosity data of mono-solvents.

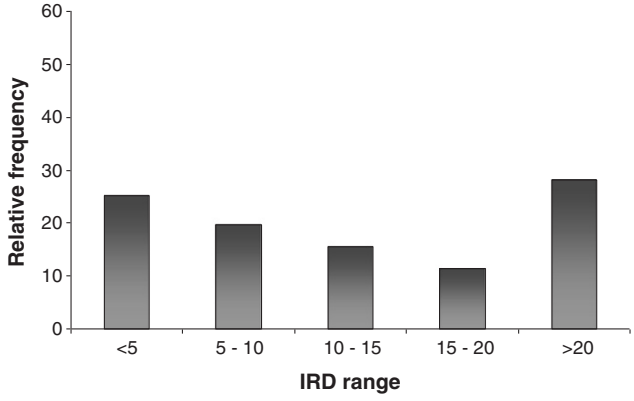

Fig. 2. The relative frequency of individual relative deviations (IRD) for predicted viscosity of binary mixtures using Eq. (7), *ab inito* prediction of viscosity of binary solvents at various temperatures.

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Table 3
List of solvents and temperature of the measured viscosity (T), experimental (Exp), calculated (Calc), d_{rs} and IRD of the calculation.

No.	Solvent	T/K	N	Ref	Exp	Calc	IRD	d_{rs}	(Exp−Calc)
1	(S)-(-)-limonene	298	1	[8]	0.846	0.865	2	0.2	−0.019
2	1-Bromobutane	308	1	[9]	0.524	0.428	18	2.0	0.096
3	1-Bromopentane	308	1	[9]	0.651	0.501	23	2.6	0.150
4	1-Bromopropane	308	1	[9]	0.440	0.362	18	2.0	0.078
5	1-Butanol	293	1	[13]	2.825	2.928	4	0.4	−0.103
6	1-Butanol	298	4	[10,11,17,19]	2.586	2.512	3	0.3	0.074
7	1-Butanol	303	5	[11,13,17,18,20]	2.272	2.166	5	0.5	0.106
8	1-Butanol	308	4	[11,17,20,22]	1.983	1.876	5	0.6	0.106
9	1-Butanol	313	3	[14,20,21]	1.794	1.633	9	0.9	0.161
10	1-Butanol	318	1	[20]	1.488	1.427	4	0.4	0.061
11	1-Chlorobutane	298	1	[29]	0.421	0.441	5	0.5	−0.020
12	1-Chlorobutane	313	1	[29]	0.364	0.312	14	1.6	0.052
13	1-Chloronaphthalene	298	1	[10]	2.806	2.234	20	2.3	0.572
14	1-Chloronaphthalene	303	1	[10]	2.487	1.930	22	2.5	0.557
15	1-Chloronaphthalene	308	1	[10]	2.214	1.675	24	2.8	0.539
16	1-Decanol	298	1	[14]	11.782	9.977	15	1.7	1.805
17	1-Decanol	303	1	[15]	8.843	8.408	5	0.5	0.435
18	1-Decanol	308	1	[14]	8.112	7.126	12	1.3	0.986
19	1-Decanol	313	1	[14]	6.819	6.071	11	1.2	0.748
20	1-Dodecanol	303	1	[15]	12.954	12.385	4	0.5	0.569
21	1-Heptanol	298	1	[14]	5.726	5.349	7	0.7	0.377
22	1-Heptanol	303	2	[14,21]	4.913	4.555	7	0.8	0.358
23	1-Heptanol	308	1	[14]	4.333	3.898	10	1.1	0.435
24	1-Heptanol	313	1	[21]	3.579	3.353	6	0.7	0.226
25	1-Hexanol	298	1	[16]	4.590	4.235	8	0.8	0.355
26	1-Hexanol	308	1	[14]	3.364	3.110	8	0.8	0.254
27	1-Hexanol	313	1	[14]	2.920	2.685	8	0.8	0.235
28	1-Nonanol	303	1	[15]	7.376	6.949	6	0.6	0.427
29	1-Octanol	298	1	[24]	7.422	6.619	11	1.1	0.803
30	1-Octanol	303	2	[14,21]	6.274	5.616	10	1.1	0.658
31	1-Octanol	308	1	[24]	5.599	4.791	14	1.6	0.808
32	1-Octanol	313	1	[14]	4.604	4.108	11	1.1	0.496
33	1-Pentanol	298	4	[16,17,25,26]	3.463	3.323	4	0.4	0.140
34	1-Pentanol	303	4	[14,15,17,25]	2.936	2.852	3	0.3	0.085
35	1-Pentanol	308	3	[10,14,17]	2.637	2.459	7	0.7	0.178
36	1-Pentanol	313	2	[14,21]	2.330	2.131	9	0.9	0.198
37	1-Propanol	293	1	[28,65]	2.171	2.090	4	0.4	0.081
38	1-Propanol	298	4	[22,25,26,65]	1.941	1.814	7	0.7	0.127
39	1-Propanol	303	5	[15,25,27,28]	1.726	1.572	9	0.9	0.154
40	1-Propanol	308	4	[10,12,18,22]	1.509	1.365	9	1.0	0.143
41	1-Propanol	313	3	[14,21,28]	1.367	1.198	12	1.3	0.169
42	1-Propanol	318	1	[65]	1.185	1.040	12	1.3	0.145
43	1,1,2,2-Tetrachloroethane	298	1	[24]	1.609	1.948	21	1.9	−0.339
44	1,1,2,2-Tetrachloroethane	308	1	[24]	1.398	1.467	5	0.5	−0.069
45	1,2-Dichloroethane	298	1	[24]	0.779	0.472	39	5.0	0.307
46	1,2-Dichloroethane	308	1	[24]	0.694	0.373	46	6.2	0.321
47	1,3-Dioxolane	288	1	[30]	0.667	0.667	0	0.0	0.000
48	1,3-Dioxolane	298	1	[29]	0.592	0.517	13	1.4	0.075
49	1,3-Dioxolane	308	1	[30]	0.535	0.406	24	2.8	0.129
50	1,3-Dioxolane	313	1	[29]	0.498	0.363	27	3.2	0.135
51	1,4-Dioxane	298	3	[10,14,29]	1.150	0.539	53	7.6	0.611
52	1,4-Dioxane	303	1	[10]	1.086	0.476	56	8.2	0.610
53	1,4-Dioxane	308	1	[10]	0.999	0.423	58	8.6	0.576
54	1,4-Dioxane	313	1	[29]	0.930	0.377	59	9.0	0.553
55	1,8-Cineole	298	1	[8]	2.556	1.145	55	8.0	1.411
56	2-(2-Methoxyethoxy)ethanol	293	1	[33]	3.906	4.580	17	1.6	−0.674
57	2-(2-Methoxyethoxy)ethanol	298	1	[33]	3.574	3.900	9	0.9	−0.326
58	2-(2-Methoxyethoxy)ethanol	303	1	[33]	3.152	3.338	6	0.6	−0.186
59	2-[2-(2-Methoxyethoxy)ethoxy]ethanol	293	1	[33]	7.211	8.041	12	1.1	−0.830
60	2-[2-(2-Methoxyethoxy)ethoxy]ethanol	298	1	[33]	6.254	6.782	8	0.8	−0.528
61	2-[2-(2-Methoxyethoxy)ethoxy]ethanol	303	1	[33]	5.412	5.752	6	0.6	−0.340
62	2-Butanol	293	2	[34,36]	3.628	2.973	18	2.0	0.655
63	2-Butanol	298	2	[19,36]	3.023	2.538	16	1.8	0.485
64	2-Butanol	303	2	[35,36]	2.495	2.197	12	1.3	0.297
65	2-Butanol	308	1	[34]	2.054	1.903	7	0.8	0.151
66	2-Butanol	313	1	[35]	1.785	1.656	7	0.8	0.129
67	2-Butanol	323	1	[35]	1.315	1.270	3	0.4	0.045
68	2-Butanone	293	2	[34,68]	0.400	0.634	59	4.6	−0.234
69	2-Butanone	298	2	[34,68]	0.330	0.558	73	5.4	−0.228
70	2-Butanone	303	2	[34,68]	0.315	0.493	60	4.6	−0.178
71	2-Butanone	308	1	[34]	0.260	0.438	68	5.2	−0.178
72	2-Butanone	313	1	[34]	0.255	0.390	53	4.3	−0.135
73	2-Chlorobutane	298	1	[29]	0.394	0.435	10	1.0	−0.041
74	2-Chlorobutane	313	1	[29]	0.337	0.308	9	0.9	0.029

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Table 3 (*continued*)

No.	Solvent	T/K	N	Ref	Exp	Calc	IRD	d_{rs}	(Exp−Calc)
75	2-Chloroethanol	298	1	[10]	2.810	2.795	1	0.1	0.015
76	2-Chloroethanol	303	1	[10]	2.448	2.405	2	0.2	0.043
77	2-Chloroethanol	308	1	[10]	2.150	2.080	3	0.3	0.070
78	2-Heptanol	298	1	[37]	5.346	5.359	0	0.0	−0.013
79	2-Hexanol	298	1	[37]	4.204	4.292	2	0.2	−0.088
80	2-Methoxyethanol	293	1	[33]	1.708	2.351	38	3.2	−0.643
81	2-Methoxyethanol	298	1	[33]	1.544	2.024	31	2.7	−0.480
82	2-Methoxyethanol	303	1	[33]	1.404	1.751	25	2.2	−0.347
83	2-Methoxyethanol	308	1	[69]	1.315	1.522	16	1.5	−0.207
84	2-Methoxyethanol	313	1	[69]	1.200	1.329	11	1.0	−0.129
85	2-Methoxyethanol	318	1	[69]	1.098	1.166	6	0.6	−0.068
86	2-Methyl-1-propanol	293	2	[34,39]	3.394	2.973	17	1.9	0.421
87	2-Methyl-1-propanol	298	2	[18,34]	3.214	2.549	21	2.3	0.664
88	2-Methyl-1-propanol	303	3	[18,34,39]	2.537	2.197	15	1.7	0.339
89	2-Methyl-1-propanol	308	2	[18,34]	2.335	1.903	18	2.0	0.432
90	2-Methyl-1-propanol	313	2	[34,39]	1.809	1.656	8	0.9	0.153
91	2-Methyl-1-propanol	323	1	[35]	1.602	1.270	21	2.3	0.332
92	2-Methyl-2-butanol	293	1	[34]	5.108	3.731	27	3.1	1.377
93	2-Methyl-2-butanol	298	1	[34]	4.474	3.188	29	3.4	1.286
94	2-Methyl-2-butanol	303	1	[34]	3.909	2.738	30	3.6	1.171
95	2-Methyl-2-butanol	308	1	[34]	3.387	2.363	30	3.6	1.024
96	2-Methyl-2-butanol	313	1	[34]	2.909	2.049	30	3.5	0.860
97	2-Methyl-2-chloropropane	298	1	[29]	0.475	0.414	13	1.4	0.061
98	2-Methyl-2-chloropropane	313	1	[29]	0.391	0.293	25	2.9	0.098
99	2-Methylpropan-2-ol	298	1	[20]	4.345	2.446	44	5.8	1.899
100	2-Methylpropan-2-ol	303	2	[20,35]	3.377	2.110	38	4.7	1.267
101	2-Methylpropan-2-ol	308	1	[20]	2.645	1.829	31	3.7	0.816
102	2-Methylpropan-2-ol	313	2	[20,35]	2.099	1.592	24	2.8	0.507
103	2-Methylpropan-2-ol	318	1	[20]	1.635	1.392	15	1.6	0.243
104	2-Methylpropan-2-ol	323	1	[35]	1.409	1.222	13	1.4	0.187
105	2-Octanol	298	1	[37]	6.568	6.671	2	0.2	−0.103
106	2-Octanol	303	1	[15]	4.804	5.660	18	1.6	-0.856
107	2-Pentanol	298	1	[15]	3.421	3.329	3	0.3	0.092
108	2-Pentanol	303	1	[15]	2.887	2.857	1	0.1	0.030
109	2-Pentanone	293	1	[68]	0.496	0.710	43	3.6	−0.214
110	2-Pentanone	298	1	[68]	0.469	0.624	33	2.9	−0.155
111	2-Pentanone	303	1	[68]	0.444	0.550	24	2.2	−0.106
112	2-Propanol	288	1	[30]	2.849	2.510	12	1.3	0.339
113	2-Propanol	293	2	[28,34]	2.163	2.153	3	0.3	0.010
114	2-Propanol	298	4	[17,18,34,37]	2.031	1.856	9	0.9	0.175
115	2-Propanol	303	4	[11,15,28,34]	1.690	1.608	8	0.9	0.081
116	2-Propanol	308	3	[17,18,34]	1.526	1.400	8	0.9	0.125
117	2-Propanol	313	2	[28,34]	1.239	1.224	9	0.9	0.014
118	2,2,4-Trimethylpentane	288	1	[30]	0.537	0.745	39	3.3	−0.208
119	2,2,4-Trimethylpentane	298	2	[30,61]	0.458	0.574	26	2.3	−0.116
120	2,2,4-Trimethylpentane	308	1	[30]	0.434	0.450	4	0.4	−0.016
121	3-Methyl-1-butanol	298	3	[11,17,18]	3.483	3.329	15	1.5	0.155
122	3-Methyl-1-butanol	303	3	[1117,18]	2.927	2.857	17	1.7	0.070
123	3-Methyl-1-butanol	308	3	[11,17,18]	2.051	2.464	36	3.0	−0.413
124	Acetone	293	1	[68]	0.320	0.588	84	6.1	−0.268
125	Acetone	298	2	[32,40]	0.309	0.518	68	5.2	−0.210
126	Acetone	303	1	[68]	0.292	0.459	57	4.5	−0.167
127	Acetonitrile	298	1	[32]	0.341	0.481	41	3.4	−0.140
128	Acetophenone	308	1	[70]	1.351	1.015	25	2.9	0.336
129	Acrylonitrile	298	1	[25]	0.341	0.583	71	5.4	−0.242
130	Acrylonitrile	303	1	[25]	0.325	0.515	58	4.6	−0.190
131	Acrylonitrile	308	1	[25]	0.311	0.457	47	3.8	−0.146
132	alfa-Pinene	298	2	[8,41]	1.293	0.854	34	4.2	0.439
133	Aniline	298	1	[41]	3.690	4.484	22	2.0	−0.794
134	Aniline	303	1	[41]	3.190	3.829	20	1.8	−0.639
135	Aniline	308	1	[41]	2.800	3.287	17	1.6	−0.487
136	Aniline	313	1	[41]	2.420	2.835	17	1.6	−0.415
137	Anisole	293	1	[42]	1.085	0.996	8	0.9	0.089
138	Anisole	298	1	[42]	1.017	0.874	14	1.5	0.143
139	Anisole	303	1	[42]	0.919	0.767	17	1.8	0.152
140	Anisole	308	1	[11]	0.855	0.677	21	2.3	0.178
141	Anisole	313	1	[35]	0.786	0.599	24	2.7	0.187
142	Anisole	323	1	[35]	0.691	0.471	32	3.8	0.220
143	Benzene	298	2	[43,56]	0.603	0.661	10	0.9	−0.058
144	Benzene	303	2	[15,46]	0.562	0.582	4	0.4	−0.021
145	Benzene	308	2	[43,50]	0.525	0.515	2	0.2	0.009
146	Benzene	313	1	[56]	0.500	0.458	8	0.9	0.042
147	Benzene	318	1	[56]	0.449	0.409	9	1.0	0.040
148	Benzonitrile	303	1	[12]	1.148	1.063	7	0.8	0.085
149	Benzonitrile	308	1	[12]	1.063	0.931	12	1.3	0.132
150	Benzoyl chloride	303	1	[46]	1.244	1.339	8	0.7	−0.095
151	Benzyl alcohol	303	1	[46]	4.504	6.209	38	3.2	−1.705

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Table 3 (*continued*)

No.	Solvent	T/K	N	Ref	Exp	Calc	IRD	d_{rs}	(Exp−Calc)
152	beta-Pinene	298	1	[8]	1.593	0.816	49	6.7	0.777
153	Bromobenzene	293	1	[47]	1.164	1.200	3	0.3	−0.036
154	Bromobenzene	303	1	[47]	0.984	0.914	7	0.7	0.070
155	Bromobenzene	313	1	[47]	0.879	0.708	19	2.2	0.171
156	Bromoform	298	1	[10]	1.977	1.459	26	3.0	0.518
157	Bromoform	303	1	[10]	1.857	1.269	32	3.8	0.588
158	Bromoform	308	1	[10]	1.733	1.109	36	4.5	0.624
159	Butyl acetate	298	1	[10]	0.669	0.633	5	0.6	0.036
160	Butyl acetate	303	1	[10]	0.627	0.558	11	1.2	0.069
161	Butyl acetate	308	1	[10]	0.589	0.494	16	1.8	0.095
162	Butylamine	293	1	[13]	0.616	2.222	261	12.8	−1.606
163	Butylamine	303	2	[13,49]	0.490	1.658	241	12.2	−1.168
164	Butylamine	313	2	[13,49]	0.431	1.261	195	10.8	−0.830
165	Butylamine	323	1	[49]	0.333	0.965	190	10.6	−0.632
166	Chlorobenzene	293	1	[47]	0.843	0.975	16	1.5	−0.132
167	Chlorobenzene	303	2	[46,47]	0.718	0.748	4	0.4	−0.030
168	Chlorobenzene	313	1	[47]	0.625	0.583	7	0.7	0.042
169	Chloroform	298	3	[10,22,32]	0.555	0.708	28	2.4	−0.153
170	Chloroform	303	1	[10]	0.534	0.624	17	1.6	−0.090
171	Chloroform	308	2	[10,22]	0.513	0.551	7	0.7	−0.038
172	Chloroform	313	1	[14]	0.491	0.489	0	0.0	0.002
173	Cyclohexane	298	1	[48]	0.899	0.468	48	6.5	0.431
174	Cyclohexane	303	1	[15]	0.821	0.416	49	6.8	0.405
175	Cyclohexane	308	1	[9]	0.737	0.370	50	6.9	0.367
176	Cyclohexanol	303	1	[45]	41.078	3.500	91	24.6	37.578
177	Decane	293	1	[36]	0.914	0.983	8	0.7	−0.069
178	Decane	298	1	[36]	0.848	0.859	1	0.1	−0.011
179	Decane	303	1	[36]	0.789	0.754	4	0.5	0.035
180	Di-n-butylamine	303	1	[49]	0.759	1.568	107	7.3	−0.809
181	Di-n-butylamine	313	1	[49]	0.657	1.194	82	6.0	−0.537
182	Di-n-butylamine	323	1	[49]	0.557	0.925	66	5.1	−0.368
183	Dibutyl ether	298	1	[50]	0.641	0.704	10	0.9	−0.063
184	Dibutyl ether	308	1	[50]	0.590	0.548	7	0.7	0.042
185	Dimethoxyethane	298	1	[16]	0.417	0.480	15	1.4	−0.063
186	Dimethylformamide	278	1	[53]	0.984	1.563	59	4.6	−0.579
187	Dimethylformamide	283	1	[53]	0.941	1.344	43	3.6	−0.403
188	Dimethylformamide	293	1	[53]	0.854	1.011	18	1.7	−0.157
189	Dimethylformamide	298	2	[10,32]	0.811	0.882	9	0.8	−0.071
190	Dimethylformamide	303	1	[10]	0.766	0.774	1	0.1	−0.008
191	Dimethylformamide	308	1	[10]	0.722	0.682	6	0.6	0.040
192	Dimethysulfoxide	298	2	[10,56]	1.914	1.210	37	4.6	0.704
193	Dimethysulfoxide	303	1	[56]	1.789	1.056	41	5.3	0.733
194	Dimethysulfoxide	308	1	[56]	1.622	0.925	43	5.6	0.697
195	Dimethysulfoxide	313	1	[56]	1.499	0.815	46	6.1	0.684
196	Dimethysulfoxide	318	1	[56]	1.381	0.720	48	6.5	0.661
197	Dodecane	293	1	[42]	1.487	1.408	5	0.5	0.079
198	Dodecane	298	1	[42]	1.450	1.223	16	1.7	0.227
199	Dodecane	303	1	[42]	1.373	1.067	22	2.5	0.306
200	Ethanol	293	1	[65]	1.202	1.377	15	1.4	−0.175
201	Ethanol	294	1	[66]	1.214	1.316	8	0.8	−0.102
202	Ethanol	298	2	[22,32]	1.084	1.196	10	1.0	−0.113
203	Ethanol	303	3	[15,17,18]	0.983	1.044	6	0.6	−0.061
204	Ethanol	308	4	[12,15,17,18]	0.892	0.912	2	0.2	−0.020
205	Ethanol	313	1	[39]	0.789	0.806	2	0.2	−0.017
206	Ethanol	318	1	[65]	0.760	0.701	8	0.8	0.059
207	Ethenylbenzene	298	1	[10]	0.708	0.894	26	2.3	−0.186
208	Ethenylbenzene	303	1	[10]	0.663	0.784	18	1.7	−0.121
209	Ethenylbenzene	308	1	[10]	0.623	0.691	11	1.0	−0.068
210	Ethyl acetate	298	2	[10,25]	0.444	0.507	14	1.3	−0.063
211	Ethyl acetate	303	1	[25]	0.407	0.449	10	1.0	−0.042
212	Ethyl acetate	308	1	[25]	0.387	0.399	3	0.3	−0.012
213	Ethyl ether	298	1	[32]	0.227	0.404	78	5.8	−0.177
214	Ethyl tert-butyl ether	293	1	[33]	0.532	0.550	3	0.3	−0.018
215	Ethyl tert-butyl ether	298	1	[33]	0.504	0.485	4	0.4	0.019
216	Ethyl tert-butyl ether	303	1	[33]	0.478	0.430	10	1.1	0.048
217	Ethylene glycol	298	1	[10]	15.312	8.516	44	5.9	6.796
218	Ethylene glycol	303	1	[10]	12.242	7.196	41	5.3	5.046
219	Ethylene glycol	308	1	[10]	9.945	6.113	39	4.9	3.832
220	Formamid	293	1	[65]	3.654	5.592	53	4.3	−1.938
221	Formamid	298	1	[65]	3.322	4.745	43	3.6	−1.423
222	Formamid	303	1	[65]	2.966	4.049	36	3.1	−1.083
223	Formamid	308	1	[65]	2.653	3.472	31	2.7	−0.819
224	Formamid	313	1	[65]	2.404	2.992	24	2.2	−0.588
225	Formamid	318	1	[65]	2.219	2.591	17	1.6	−0.372
226	Glycerol	294	1	[66]	1390.000	287.940	79	15.7	1102.060
227	Heptane	293	1	[42]	0.413	0.595	44	3.7	−0.182

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Table 3 (*continued*)

No.	Solvent	T/K	N	Ref	Exp	Calc	IRD	d_{rs}	(Exp−Calc)
228	Heptane	298	1	[42]	0.391	0.524	34	2.9	−0.133
229	Heptane	303	1	[42]	0.370	0.464	25	2.3	−0.094
230	Hexane	293	1	[42]	0.311	0.515	66	5.0	−0.204
231	Hexane	298	1	[42]	0.295	0.455	54	4.3	−0.160
232	Hexane	303	1	[42]	0.284	0.403	42	3.5	−0.119
233	m-Cresol	313	1	[67]	6.252	13.071	109	7.4	−6.819
234	m-Cresol	323	1	[67]	4.111	9.298	126	8.2	−5.187
235	m-Cresol	333	1	[67]	3.007	6.825	127	8.2	−3.818
236	m-Xylene	298	1	[56]	0.588	0.833	42	3.5	−0.245
237	m-Xylene	303	1	[56]	0.553	0.733	33	2.8	−0.180
238	m-Xylene	308	1	[56]	0.523	0.646	24	2.1	−0.123
239	m-Xylene	313	1	[56]	0.493	0.572	16	1.5	−0.079
240	m-Xylene	318	1	[56]	0.468	0.506	8	0.8	−0.038
241	Mesitylene	298	1	[17]	0.641	0.939	47	3.8	−0.298
242	Mesitylene	303	1	[17]	0.601	0.823	37	3.1	−0.222
243	Mesitylene	308	1	[17]	0.566	0.721	27	2.4	−0.155
244	Mesitylene	313	1	[56]	0.542	0.640	18	1.7	−0.098
245	Mesitylene	318	1	[56]	0.507	0.564	11	1.1	−0.057
246	Methanol	293	1	[47]	0.591	0.694	17	1.6	−0.103
247	Methanol	298	2	[26,52]	0.515	0.609	18	1.7	−0.094
248	Methanol	303	2	[47,49]	0.510	0.538	6	0.5	−0.028
249	Methanol	308	2	[10,12]	0.460	0.477	5	0.4	−0.017
250	Methanol	313	2	[47,49]	0.452	0.424	6	0.6	0.027
251	Methanol	323	1	[49]	0.396	0.339	14	1.6	0.057
252	Methyl acetate	298	1	[10]	0.389	0.470	21	1.9	−0.081
253	Methyl acetate	303	1	[10]	0.370	0.417	13	1.2	−0.047
254	Methyl acetate	308	1	[10]	0.353	0.371	5	0.5	−0.018
255	Methylcyclohexane	298	1	[43]	0.683	0.541	21	2.3	0.142
256	Methylcyclohexane	303	1	[43]	0.641	0.484	25	2.8	0.157
257	Methylcyclohexane	308	1	[43]	0.590	0.426	28	3.3	0.164
258	Methylcyclopentane	293	1	[68]	0.504	0.522	4	0.4	−0.018
259	Methylcyclopentane	298	1	[68]	0.476	0.461	3	0.3	0.015
260	Methylcyclopentane	303	1	[68]	0.450	0.408	9	1.0	0.042
261	N-Methylacetamide	308	2	[69,70]	3.347	2.698	19	2.2	0.649
262	N-Methylacetamide	313	1	[69]	3.004	2.334	22	2.5	0.670
263	N-Methylacetamide	318	1	[69]	2.673	2.029	24	2.8	0.644
264	N,N-dimethylacetamide	298	1	[10]	0.937	0.856	9	0.9	0.081
265	N,N-dimethylacetamide	303	1	[10]	0.878	0.752	14	1.6	0.126
266	N,N-dimethylacetamide	308	1	[10]	0.823	0.662	20	2.2	0.161
267	Nitrobenzene	298	1	[63]	1.806	1.412	22	2.5	0.394
268	Nitromethan	298	1	[63]	0.614	0.496	19	2.1	0.118
269	Nonane	293	1	[42]	0.714	0.824	15	1.4	−0.110
270	Nonane	298	1	[42]	0.672	0.722	8	0.7	−0.050
271	Nonane	303	1	[42]	0.631	0.636	1	0.1	−0.005
272	o-Cresol	313	1	[56]	4.243	13.071	208	11.3	−8.828
273	o-Cresol	323	1	[56]	3.020	9.298	208	11.3	−6.278
274	o-Cresol	333	1	[67]	2.274	6.825	200	11.0	−4.551
275	o-Xylene	298	1	[56]	0.760	0.833	10	0.9	−0.073
276	o-Xylene	303	1	[56]	0.720	0.733	2	0.2	−0.013
277	o-Xylene	308	1	[56]	0.680	0.646	5	0.5	0.034
278	o-Xylene	313	1	[56]	0.640	0.572	11	1.1	0.068
279	o-Xylene	318	1	[56]	0.598	0.506	15	1.7	0.092
280	Octane	293	1	[36]	0.542	0.701	29	2.6	−0.159
281	Octane	298	1	[36]	0.509	0.616	21	1.9	−0.107
282	Octane	303	1	[36]	0.481	0.544	13	1.2	−0.063
283	p-Cresol	313	1	[67]	6.661	12.920	94	6.6	−6.259
284	p-Cresol	323	1	[67]	4.480	9.298	108	7.3	−4.818
285	p-Cresol	333	1	[67]	3.232	6.825	111	7.5	−3.593
286	p-Cymene	298	1	[8]	0.798	1.115	40	3.4	−0.317
287	p-Xylene	298	1	[50]	0.613	0.835	36	3.1	−0.222
288	p-Xylene	303	1	[56]	0.570	0.729	28	2.5	−0.159
289	p-Xylene	308	1	[50]	0.540	0.646	20	1.8	−0.106
290	p-Xylene	313	1	[56]	0.520	0.572	10	1.0	−0.052
291	p-Xylene	318	1	[56]	0.491	0.506	3	0.3	−0.015
292	Propiophenone	308	1	[70]	1.468	1.159	21	2.4	0.309
293	Propyl acetate	298	1	[10]	0.557	0.560	0	0.1	−0.003
294	Propyl acetate	303	1	[10]	0.518	0.495	5	0.5	0.023
295	Propyl acetate	308	1	[10]	0.486	0.439	10	1.0	0.047
296	Propylbenzene	303	1	[15]	0.750	0.884	18	1.6	−0.134
297	Propylene glycol monoethyl ether	298	1	[19]	1.905	1.527	20	2.2	0.378
298	Propylene glycol monomethyl ether	298	1	[19]	1.670	1.527	9	0.9	0.143
299	Propylene glycol monopropyl ether	298	1	[19]	2.396	1.527	36	4.5	0.869
300	Propylene glycol tert-butyl ether	298	1	[19]	3.246	1.509	54	7.7	1.737
301	Pyridine	298	1	[52]	0.881	0.745	15	1.7	0.136
302	tert-Amyl methyl ether	298	1	[26]	0.438	0.485	11	1.0	−0.047
303	tert-Butyl methyl ether	298	1	[26]	0.340	0.423	24	2.2	−0.083
304	Tetrachloromethane	298	1	[74]	0.902	0.566	37	4.7	0.336

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Table 3 (*continued*)

No.	Solvent	T/K	N	Ref	Exp	Calc	IRD	d_{rs}	(Exp−Calc)
305	Tetrahydrofuran	293	1	[16]	0.480	0.486	1	0.1	−0.006
306	Tetrahydrofuran	298	1	[10]	0.472	0.430	9	0.9	0.042
307	Tetrahydrofuran	303	2	[15,16]	0.430	0.382	11	1.2	0.048
308	Tetrahydrofuran	308	1	[10]	0.429	0.340	21	2.3	0.089
309	Tetrahydrofuran	313	1	[16]	0.390	0.304	22	2.5	0.086
310	Toluene	278	1	[53]	0.665	1.271	91	6.5	−0.606
311	Toluene	283	1	[53]	0.637	1.101	73	5.5	−0.464
312	Toluene	293	1	[53]	0.578	0.833	44	3.7	−0.255
313	Toluene	298	1	[20]	0.557	0.729	31	2.7	−0.172
314	Toluene	303	1	[20]	0.527	0.641	22	2.0	−0.114
315	Toluene	308	1	[20]	0.496	0.567	14	1.4	−0.071
316	Toluene	313	1	[20]	0.466	0.503	8	0.8	−0.037
317	Toluene	318	1	[20]	0.463	0.447	3	0.4	0.016
318	Tri-n-butylamine	303	1	[21]	1.167	1.053	10	1.0	0.114
319	Tri-n-butylamine	313	1	[21]	0.997	0.807	19	2.1	0.190
320	Trichloroethane	293	1	[39]	0.572	0.572	0	0.0	0.000
321	Trichloroethane	303	1	[39]	0.532	0.446	16	1.8	0.086
322	Trichloroethane	313	1	[39]	0.473	0.354	25	2.9	0.119
323	Trichloroethylene	293	1	[39]	0.572	0.701	23	2.0	−0.129
324	Trichloroethylene	298	1	[23]	0.527	0.616	17	1.6	−0.089
325	Trichloroethylene	303	1	[39]	0.532	0.544	2	0.2	−0.012
326	Trichloroethylene	313	1	[39]	0.473	0.429	9	1.0	0.044
327	Triethylamine	303	1	[27]	0.330	0.480	45	3.8	−0.150
						Overall	27	2.5	

was calculated for the calculated data by Eq. (6) using ($d_{rms} = \sqrt{\sum\left[100\ ln\left(\frac{Experimental}{Calculated}\right)\right]^2 / N}$). The d_{rms} values of the data sets employed in this study were listed in column 9 of Table 2 in which the overall d_{rms} of 0.7 ± 0.7 (number of data sets = 580) was obtained for Eq. (6). The corresponding value for the Hildebrand fluidity equation was 2.3 ± 1.9 (number of data sets = 17). In addition to better prediction capability of our proposed model, its calculations are straightforward and could be carried out using any computational software. The next advantage of the proposed model over Hildebrand fluidity equation is that it is applicable for any solvent at any temperature of interest and the only required information is the Abraham parameters could be computed using Pharma-Algorithm software, however, there are some limitations in the application of Hildebrand fluidity equation as stated in the literature [78]. Two accuracy criteria (i.e. MRD and d_{rms}) show high correlation and for our data sets the Pearson correlation coefficient of 0.965 was obtained revealing that both criteria could present the deviations of the calculated data from experimental values.

3.2. Ab initio modeling of viscosity data

The collected η_m data of binary solvent mixtures at various temperatures were fitted to Eq. (4) and the resulted ab initio model to predict the η_m value is

$$\begin{aligned} ln\,\eta_{m,T} = {} & -7.092x_1 + \frac{x_1}{T}\left\{\begin{array}{l} 1555.445 + 117.243E_1 + 291.658S_1 + 2356.794A_1 - 766.788B_1 \\ + 375.175V_1 + 1255.266A_1\cdot B_1 - 969.034\frac{A_1}{V_1} + 480.368\frac{B_1}{V_1} \end{array}\right\} \\ & -5.344x_2 + \frac{x_2}{T}\left\{\begin{array}{l} 1236.187 + 109.280E_2 + 181.976S_2 + 9288.019A_2 + 491.210B_2 + 93.674V_2 \\ -24658.081A_2\cdot B_2 - 5490.785\frac{A_2}{V_2} - 528.355\frac{B_2}{V_2} + 17773.086\frac{A_2\cdot B_2}{V_2} \end{array}\right\} \\ & + \frac{x_1x_2}{T}\left[-250.365 + 305.706(E_1-E_2)^2 + 262.761(V_1-V_2)^2 + 748.863(B_1-B_2)^2\right] \\ & + \frac{x_1x_2(x_1-x_2)}{T}\left[-37.261 - 179.152(S_1-S_2)^2 + 1025.738(B_1-B_2)^2 - 191.113(V_1-V_2)^2\right] \\ & + \frac{x_1x_2(x_1-x_2)^2}{T}[-432.536 + 721.667(E_1-E_2)^2 + 5051.184(A_1-A_2)^2 \\ & + 1365.945(B_1-B_2)^2]. \end{aligned} \quad (7)$$

The model was statistically significant with the F value of 2042 ($p<0.0005$). The back-calculated viscosity resulted in the MRD values in the range of 2% (for methanol + acetonitrile at 298 K) and 88% (for acetone + hexane at 298 K) with the overall MRD (±SD) of 17 (±17)% (for details of the MRD values, see Table 2). Eq. (7) predicts viscosity of binary solvents at various temperatures for all fraction composition ranges from 0 to 1. Fig. 2 shows the relative frequency of IRDs in different subgroups where in more than 20% of the cases, the IRD is more than 20. This is because of the low accuracy of the model for predicting the viscosity of mono-solvents using the proposed chemical descriptors.

3.3. Prediction of viscosity for mono-solvents at various temperatures

Considering $x_1 = 1$, Eq. (4) reduces to a simpler form. The trained version of the simpler model using the mono-solvent data at various temperatures is

$$ln\,\eta_T = -8.066 + \frac{1}{T}\left\{\begin{array}{l} 1777.751 + 124.148E_1 + 251.298S_1 + 2287.788A_1 - 341.293B_1 + 360.072V_1 \\ + 853.257A_1\cdot B_1 - 699.612\frac{A_1}{V_1} + 255.149\frac{B_1}{V_1} \end{array}\right\} \quad (8)$$

which could be used to predict viscosity of mono-solvents at various temperatures (η_T). The overall MRD value of the back-calculated viscosities is 27%, and as listed in Table 3, a number of solvents, such as buthylamine, o-cresol, m-cresol and p-cresol produced very large prediction errors. By excluding these solvents, the MRD reduces to

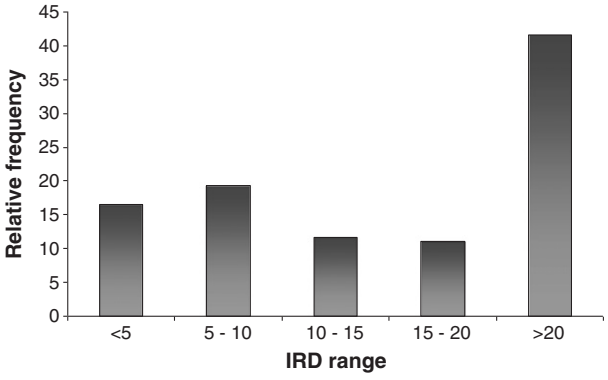

Fig. 3. The relative frequency of individual relative deviations (IRD) for predicted viscosity of binary mixtures using Eq. (8) ab initio prediction of the viscosity of mono-solvents at various temperatures.

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Table 4
List of solvents and temperature of the measured viscosity at temperature (T), and comparison of the experimental viscosities (Exp 1 and Exp 2) from references 1 and 2, and IRD of two measurements.

No.	Solvent	T/K	Exp1	Exp2	Ref 1	Ref 2	IRD
1	1-Propanol	298	2.077	1.740	[18]	[10]	19
2	1-Propanol	303	1.809	1.550	[18]	[10]	17
3	1-Propanol	308	1.595	1.380	[18]	[10]	16
4	2-Butanone	298	0.380	0.280	[68]	[34]	36
5	2-Butanone	303	0.360	0.270	[68]	[34]	33
6	2-Methyl-1-propanol	293	4.037	2.750	[34]	[39]	47
7	2-Methyl-1-propanol	303	2.875	2.100	[34]	[39]	37
8	2-Methyl-1-propanol	313	1.650	2.116	[39]	[35]	22
9	2-Propanol	313	1.347	1.000	[34]	[39]	35
10	2-Propanol	293	2.226	1.700	[34]	[39]	31
11	2-Propanol	303	1.786	1.400	[18]	[39]	28
12	3-Methyl-1-butanol	308	2.790	1.518	[17]	[11]	84
13	3-Methyl-1-butanol	303	2.258	3.261	[18]	[17]	31
14	3-Methyl-1-butanol	298	2.780	3.835	[18]	[17]	28
15	Acetone	298	0.303	0.350	[40]	[32]	13
16	Butylamine	303	0.540	0.440	[13]	[49]	23
17	Butylamine	313	0.470	0.390	[13]	[49]	21
18	Dimethylformamide	298	0.816	0.640	[10]	[59]	28
19	Dimethysulfoxide	298	1.358	1.998	[59]	[54]	32
20	Ethanol	293	1.202	1.000	[65]	[39]	20
21	Ethyl acetate	298	0.370	0.457	[32]	[10]	19
22	Nitromethane	298	0.520	0.646	[59]	[32]	20
23	o-Xylene	298	0.760	0.676	[56]	[44]	12
24	Toluene	298	0.590	0.507	[32]	[44]	16

22% and possesses an advantage of predicting viscosity at various temperatures. Considering IRD definition, when the differences between experimental and calculated viscosities were divided by experimental viscosities, the obtained value will be relatively a small when the viscosity of the solvent is high and will be a large value for low experimental viscosities. As an example, the IRD of 79% was obtained for glycerol where the experimental value of 1390.000 was calculated as 287.940. Butylamine at 293 K with the experimental and calculated viscosities of 0.616 and 2.222 is another example which produced the IRD of 261%. To provide another accuracy criterion, the term used by Bertrand [78] was also employed and the obtained d_{rs} ($d_{rs} = \sqrt{\sum \left[100\ ln\left(\frac{Experimental}{Calculated}\right)\right]^2}$) values are listed in Table 3. There is a parallel pattern between d_{rs} and IRD (Pearson correlation coefficient of 0.855) and in most of the cases, the high IRD is the high d_{rs} value. Large deviations (for both d_{rs} and IRD) could be originated from:

1) Weakness of the model for describing very high and very low viscosities
2) Possible errors in the computation of the Abraham parameters by Pharma-Algorithm software.

An alternative accuracy criterion for such cases could be a simple difference between experimental and calculated values which are listed in Table 3. Careful examination of the results and considering the difference of 0.05 as acceptable level reveal that in 17.2% of the cases, the model provides acceptable predictions, and in 34.7 and 48.1% of the cases underpredictions and overpredictions were observed, respectively.

Fig. 3 shows the relative frequency of IRDs in different subgroups where in more than 42% of the cases, the IRD is more than 20. The variations of the experimental viscosity data reported in the literature are relatively high as a number of examples are listed in Table 4. Considering the listed IRDs, the prediction error of 25 or 18% could be considered as an acceptable error since the model predicts the viscosity at various temperatures and no need for any experimental data.

4. Conclusion

Two trained versions of the Jouyban–Acree models were presented for calculation of viscosity of solvent mixtures. Eq. (6) employs two experimental viscosities of mono-solvents at the temperature of interest and produced the overall MRDs of 7%. Eq. (7) is an ab initio method and predicts the viscosity of binary solvent mixtures with the overall MRD of 17%. As briefly discussed in Introduction, knowledge of viscosity is required in many applications and data of most of the solvent mixtures are not available in the literature. The proposed model could also be employed to predict the viscosities of mono-solvents at various temperatures. Although the proposed models employ well-established descriptors to represent the effects of solvent natures, and their compositions, because of numerous curve-fitting parameters of the models, providing theoretical or semi-theoretical justifications for the models is a hard task, and we prefer to consider them as empirical models.

The proposed model provides the most accurate predictions for the viscosity of binary solvents employing viscosity of mono-solvents, and could be recommended for industrial applications, however for ab initio viscosity predictions (for binary solvents and also mono-solvents), further investigations and more improvements are required to provide more accurate predictions.

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