

# Electronic Supplementary Information

## Contact Angles and Wettability of Ionic Liquids on Polar and Non-polar Surfaces

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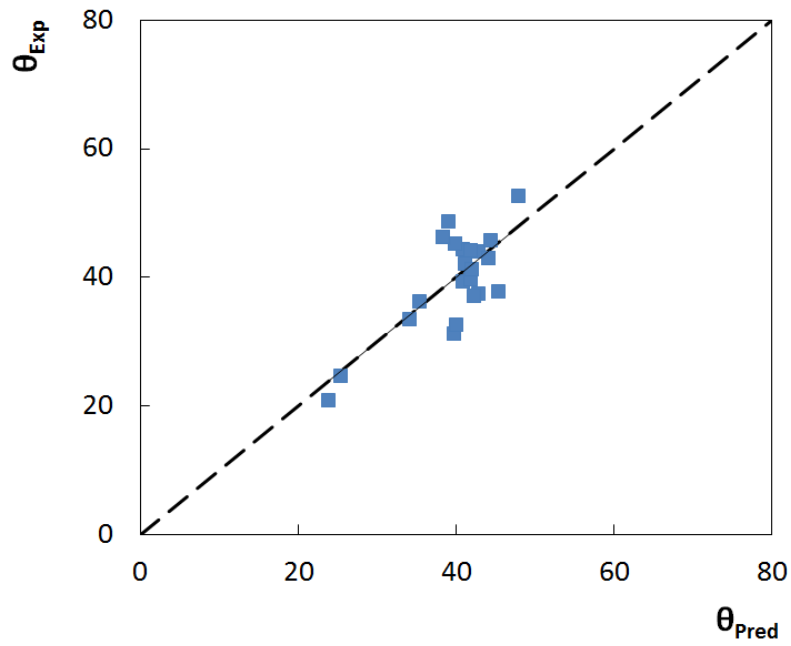


Figure S1. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S1.

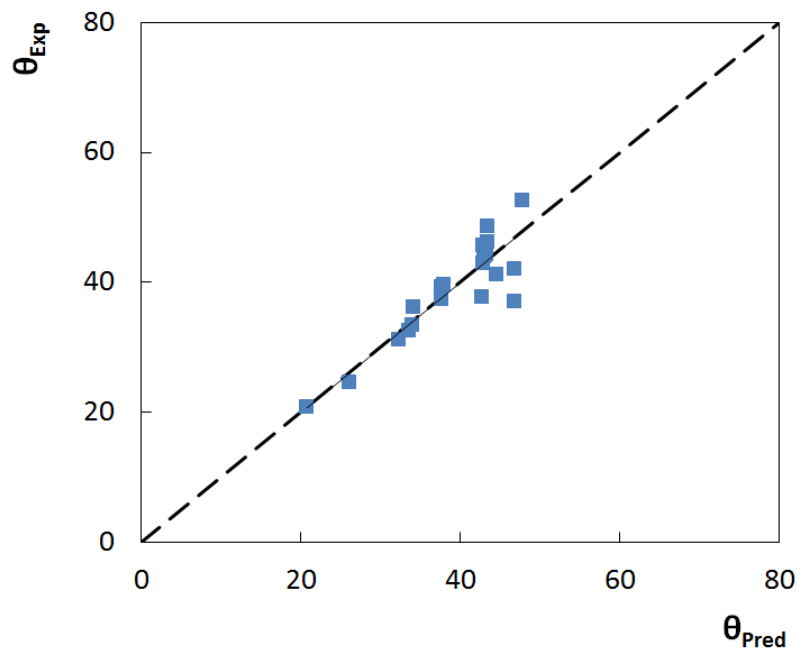


Figure S2. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation 3.

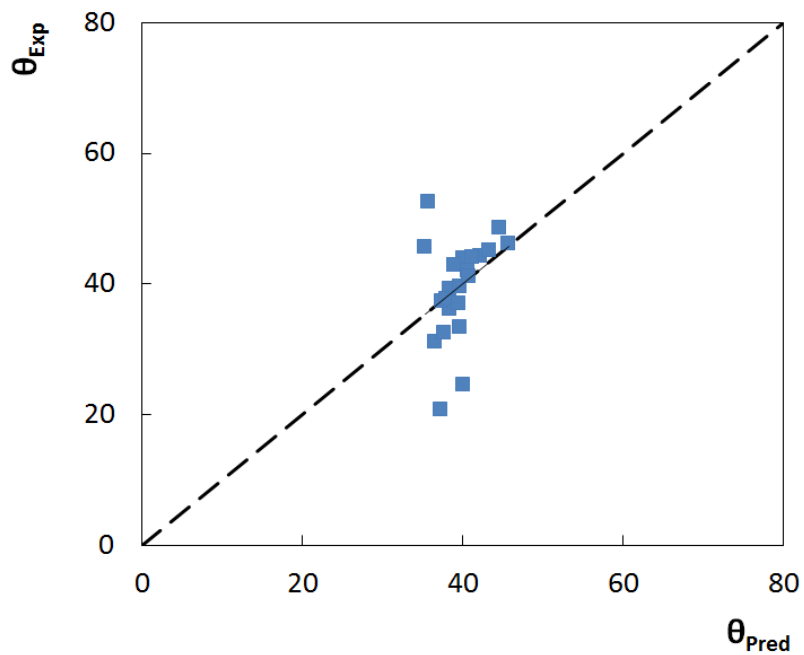


Figure S3. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S2.

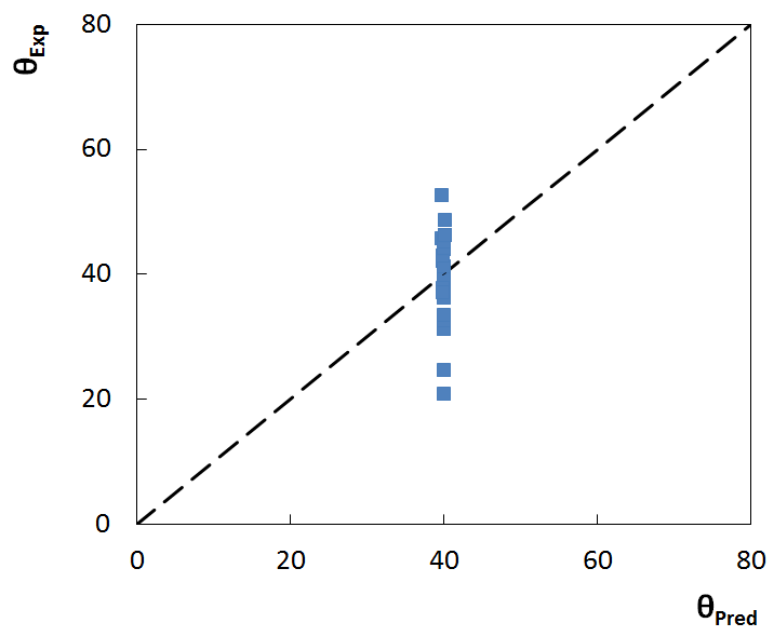


Figure S4. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S3.

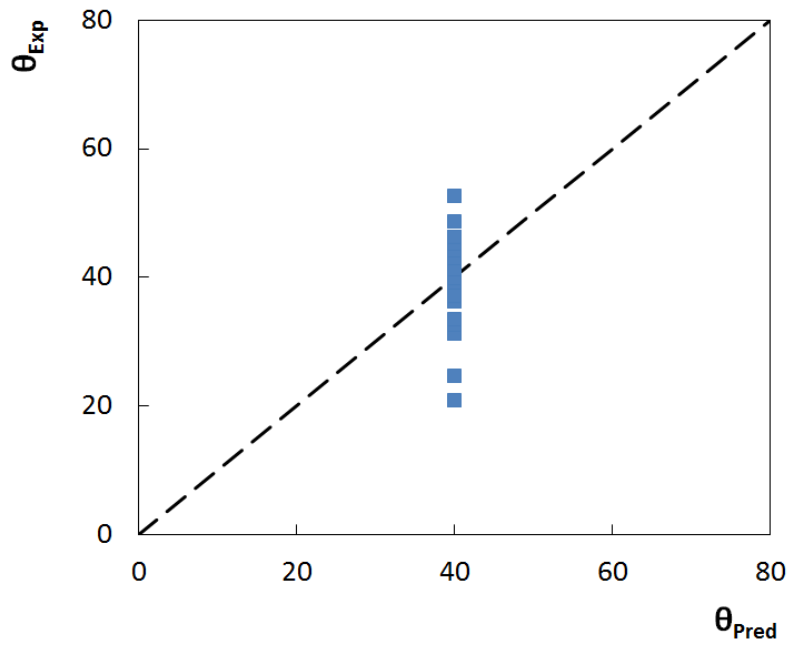


Figure S5. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S4.

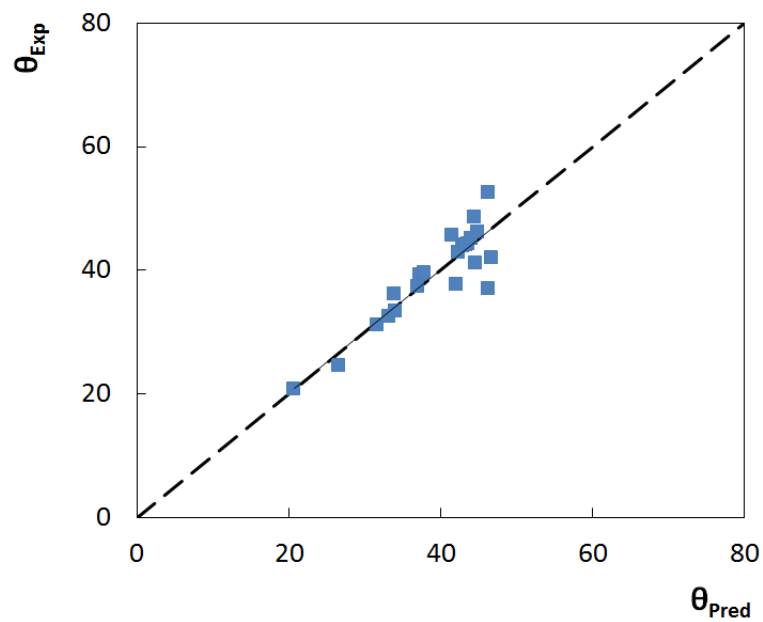


Figure S6. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S5.

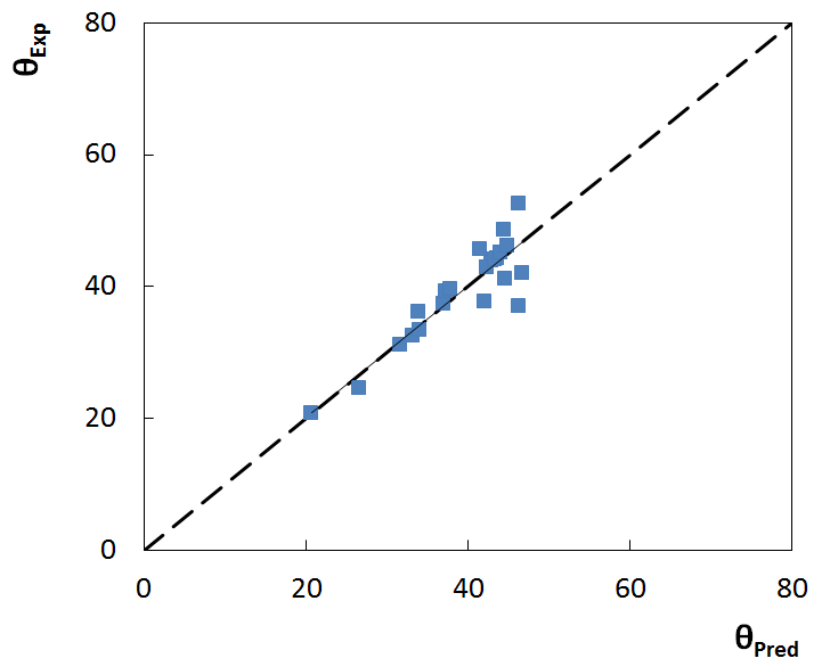


Figure S7. Comparison between experimental,  $\theta_{\text{Exp}}$ , and predictive,  $\theta_{\text{Pred}}$ , contact angles values using Equation S6.

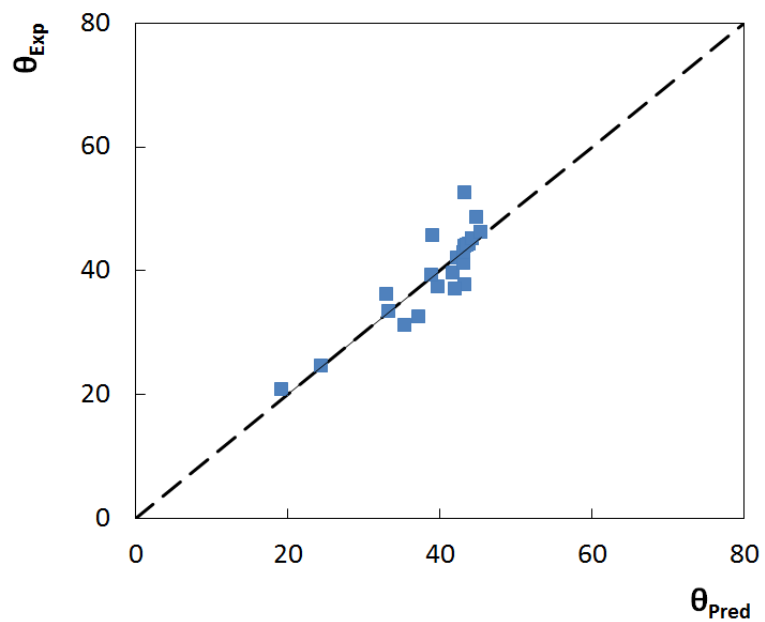


Figure S8. Comparison between experimental,  $\theta_{\text{Exp}}$ , and predictive,  $\theta_{\text{Pred}}$ , contact angles values using Equation S7.

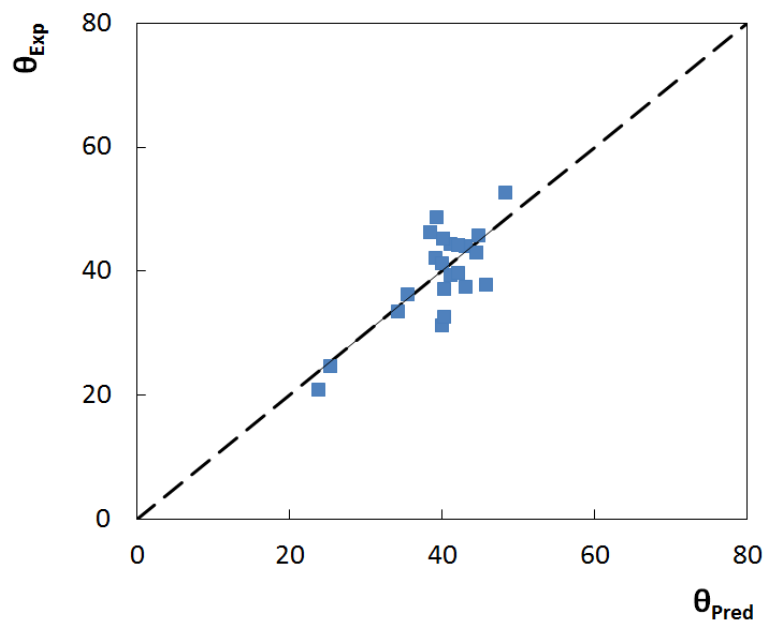


Figure S9. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S8.

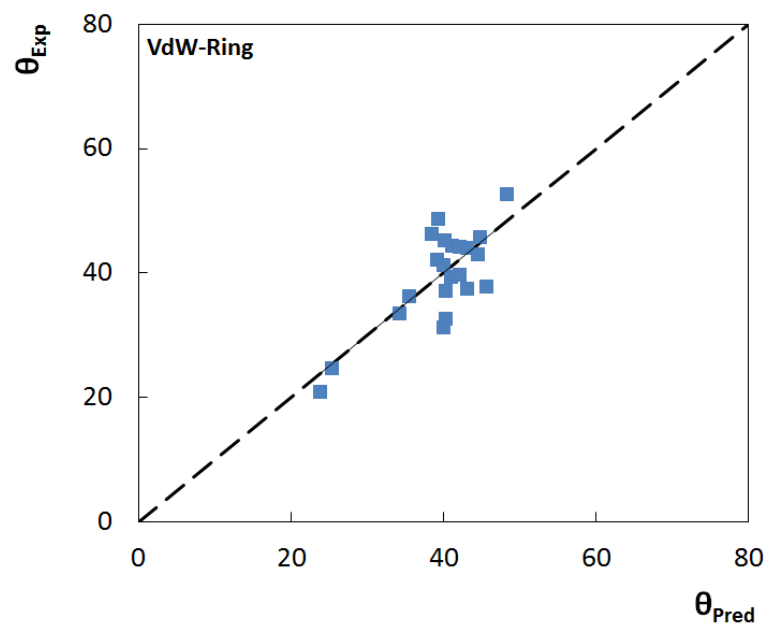


Figure S10. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S9.

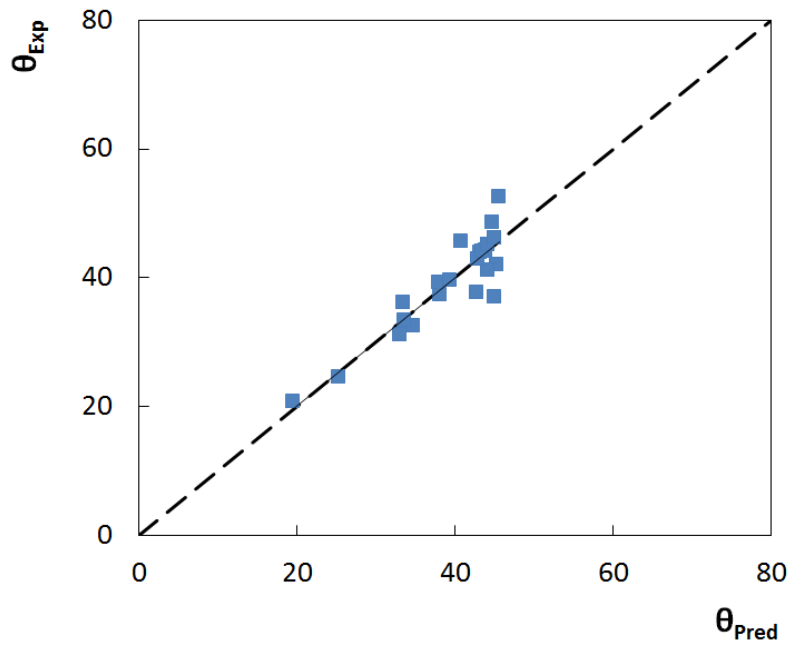


Figure S11. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S10.

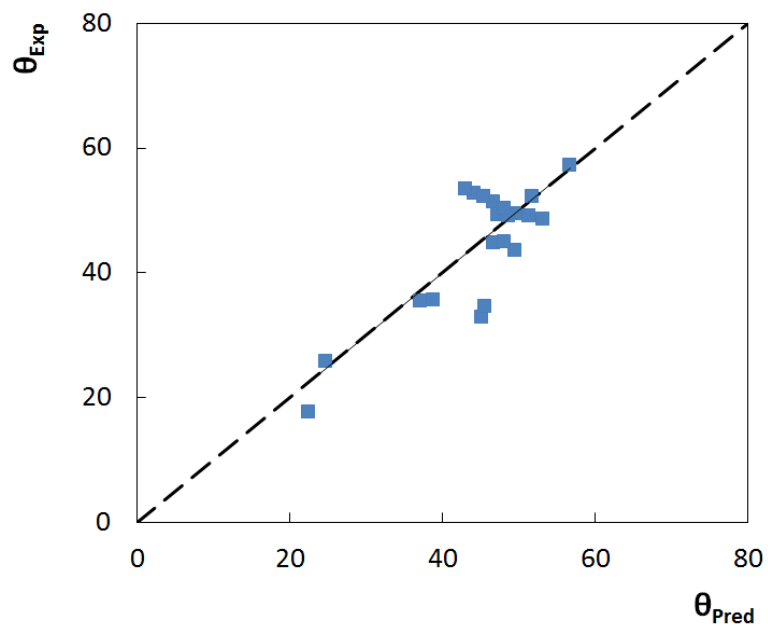


Figure S12. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S11.

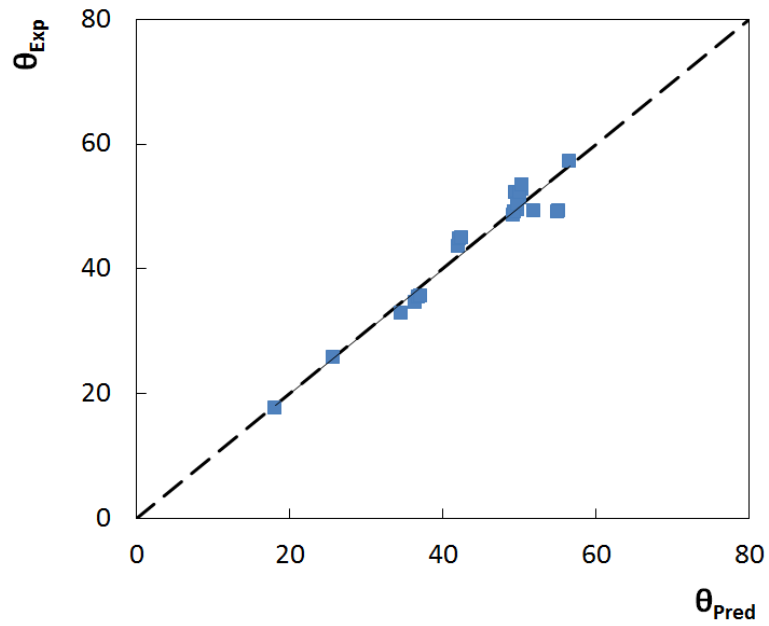


Figure S13. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation 5.

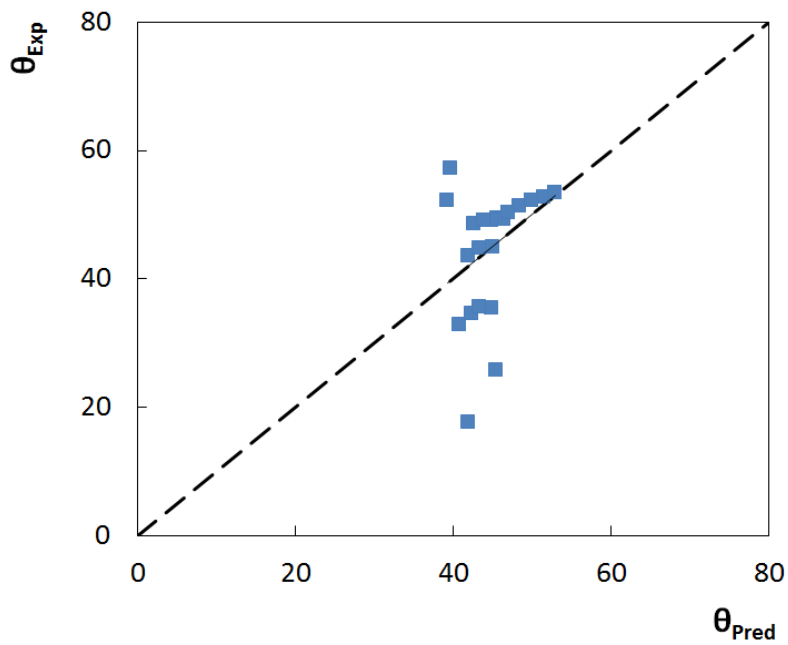


Figure S14. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S12.



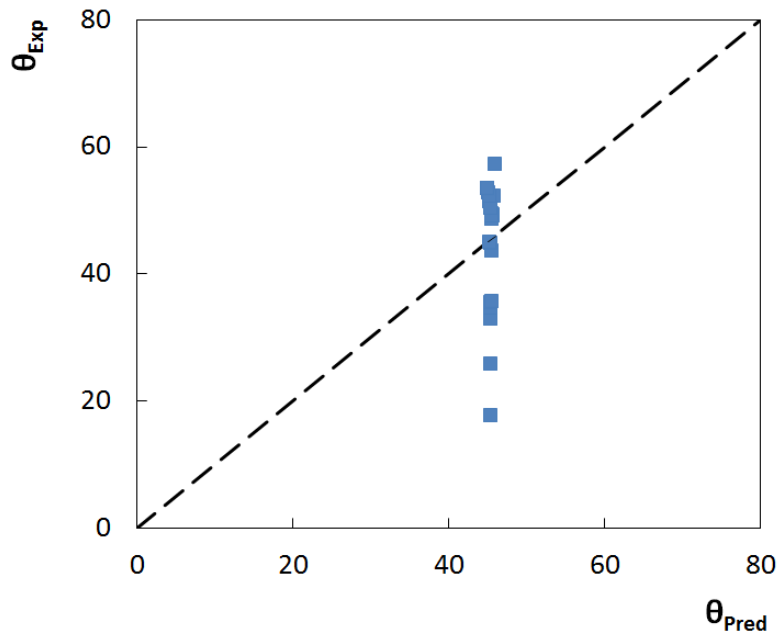


Figure S15. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S13.

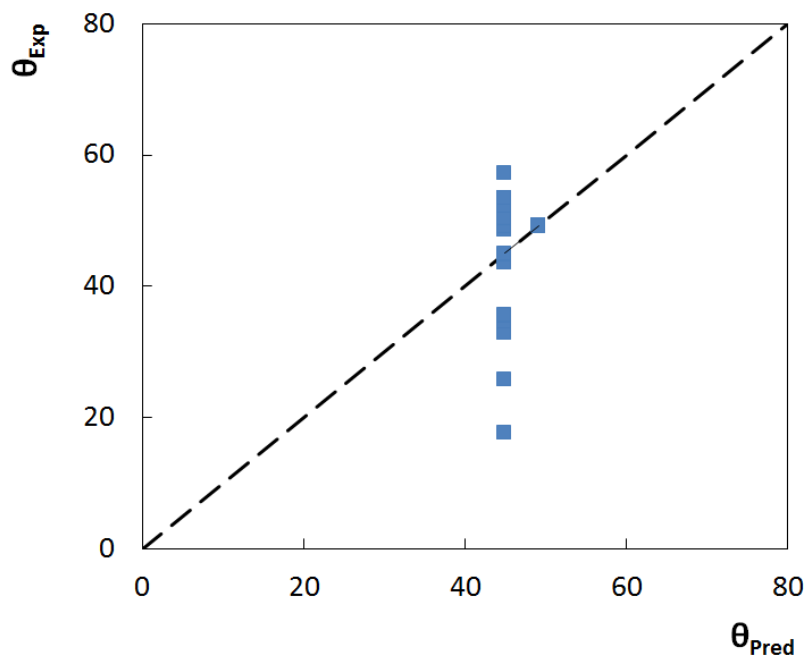


Figure S16. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S14.

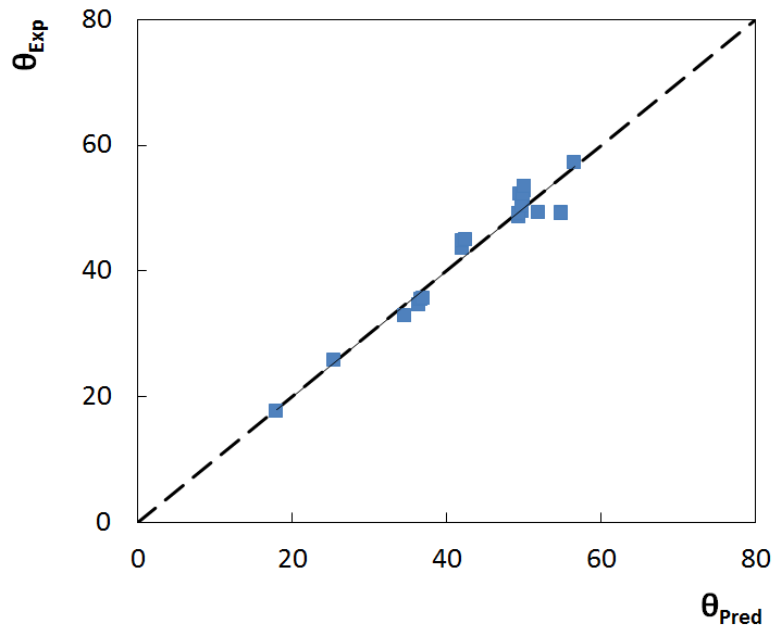


Figure S17. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S15.

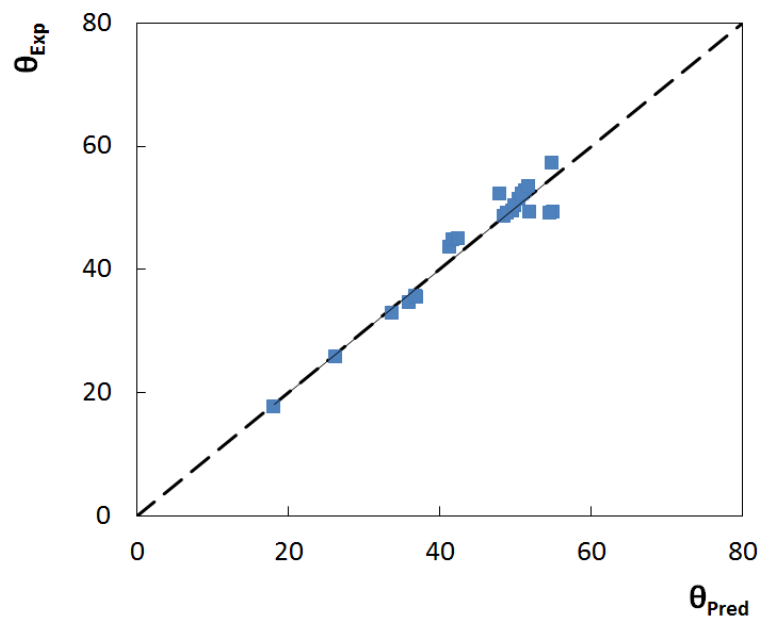


Figure S18. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S16.

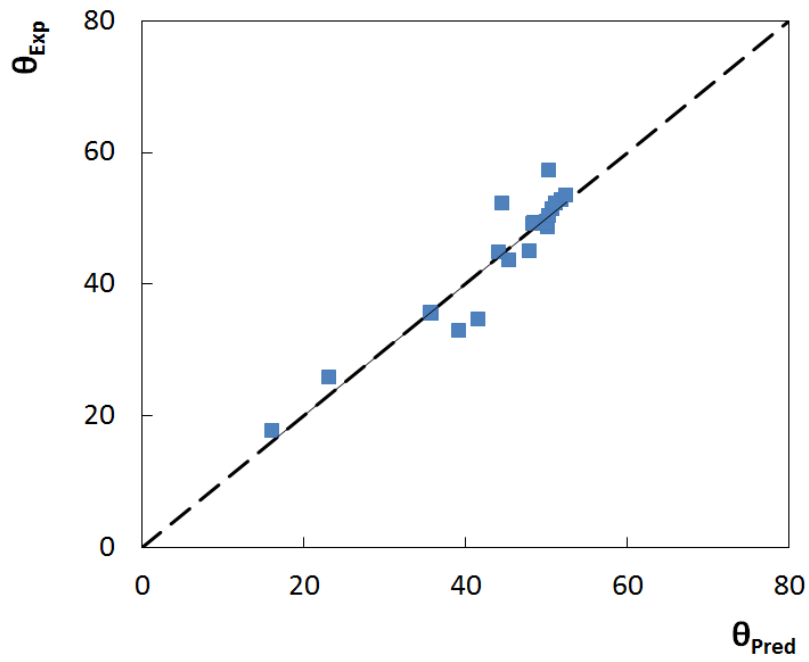


Figure S19. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S17.

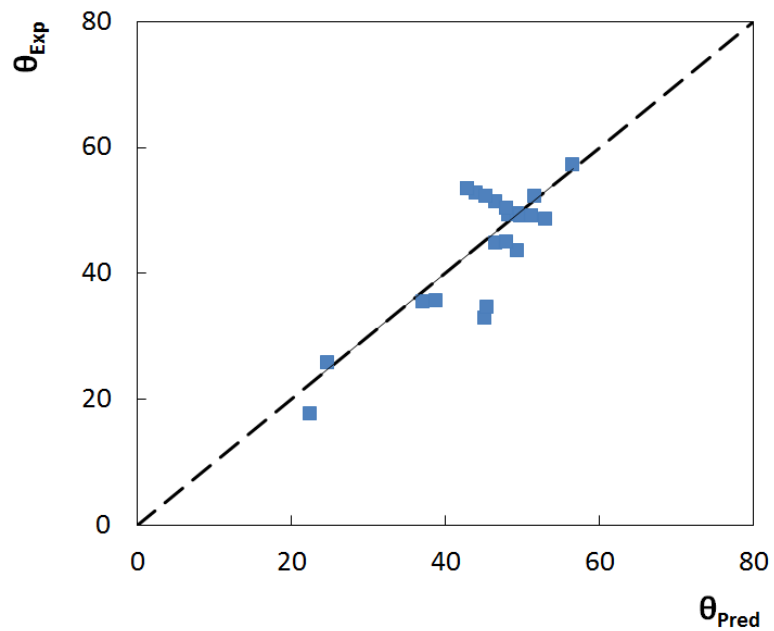


Figure S20. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S18.

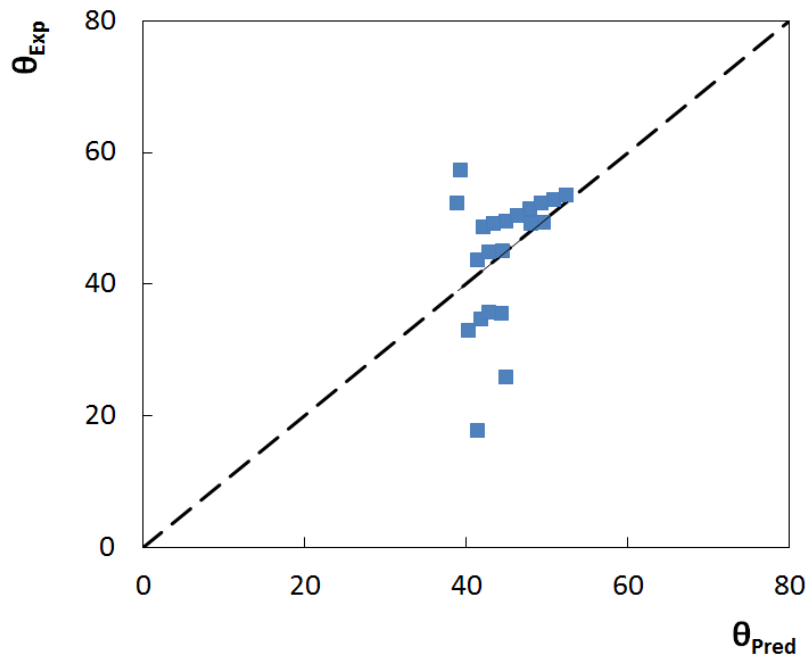


Figure S21. Comparison between experimental,  $\theta_{\text{Exp}}$ , and predictive,  $\theta_{\text{Pred}}$ , contact angles values using Equation S19.

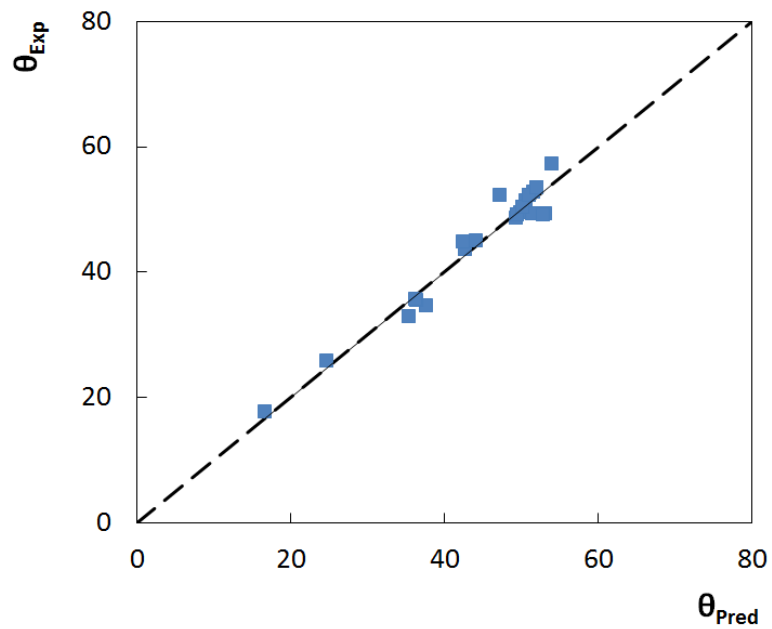


Figure S22. Comparison between experimental,  $\theta_{\text{Exp}}$ , and predictive,  $\theta_{\text{Pred}}$ , contact angles values using Equation S20.

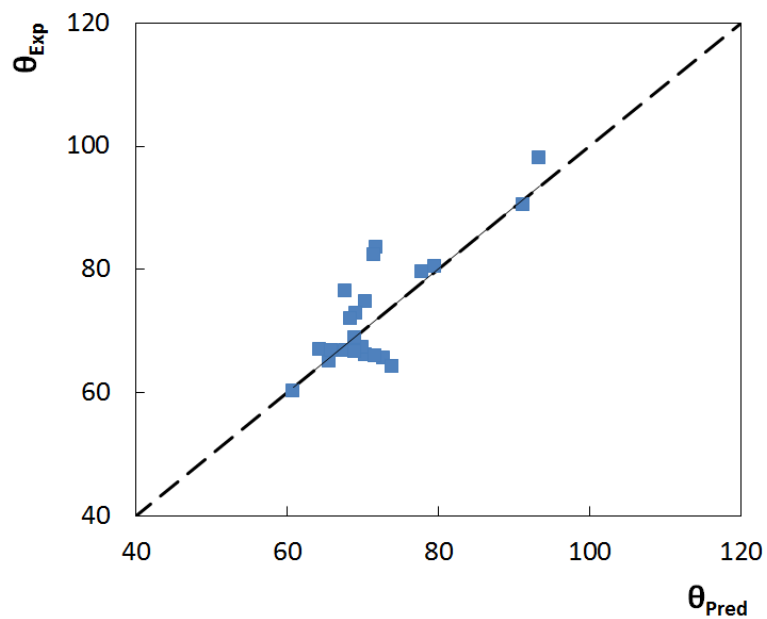


Figure S23. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S21.

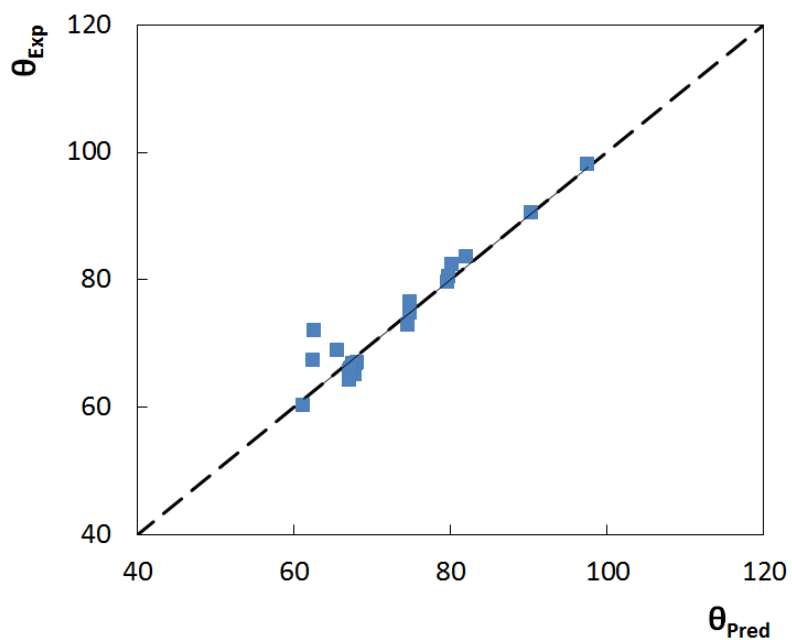


Figure S24. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation 7.

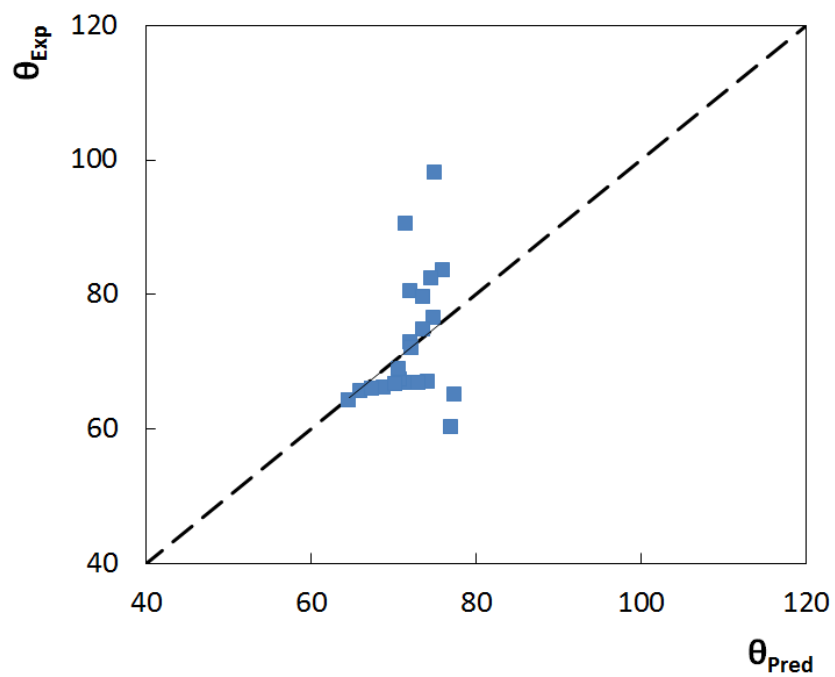


Figure S25. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S22.

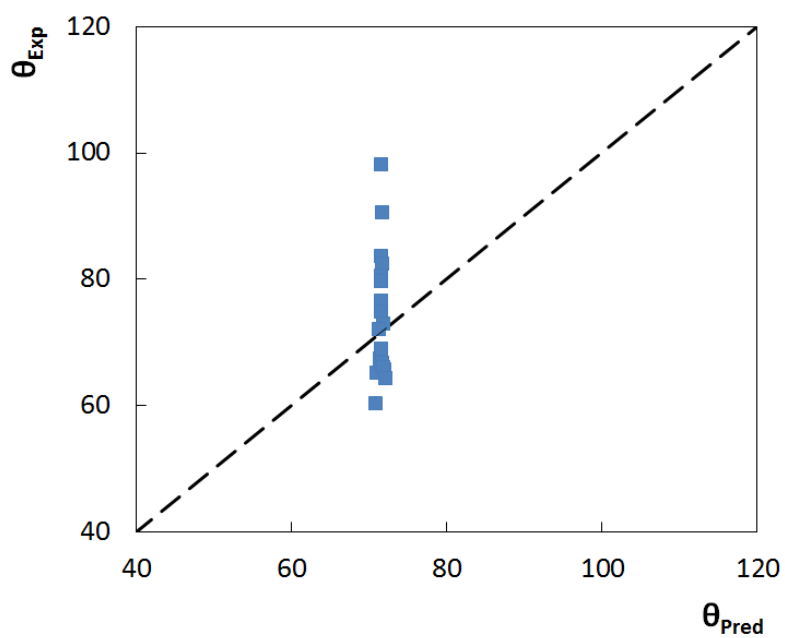


Figure S26. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S23.

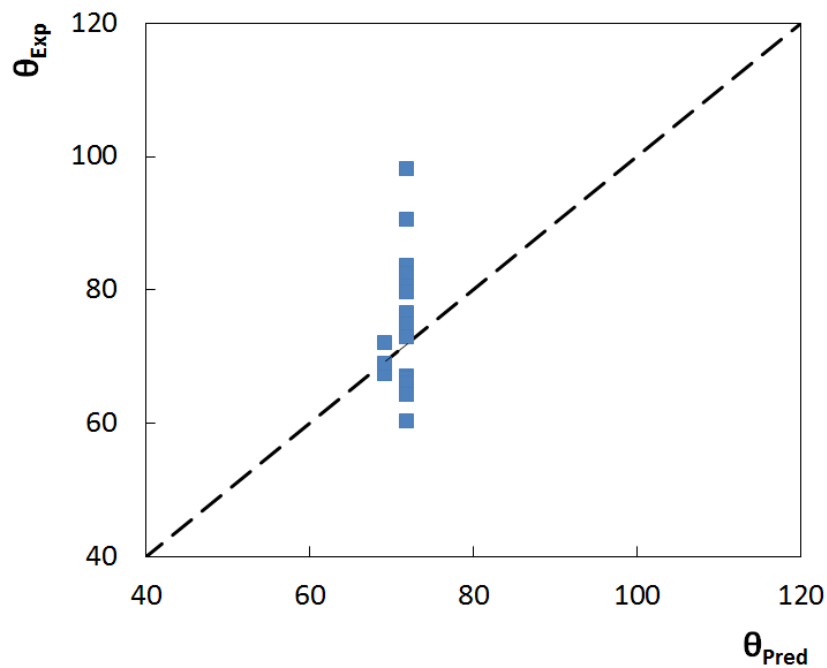


Figure S27. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S24.

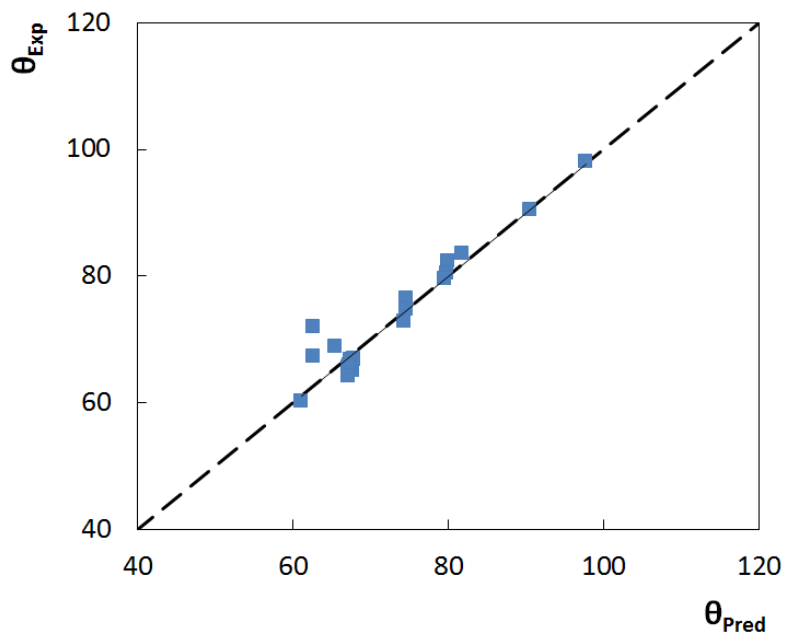


Figure S28. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S25.

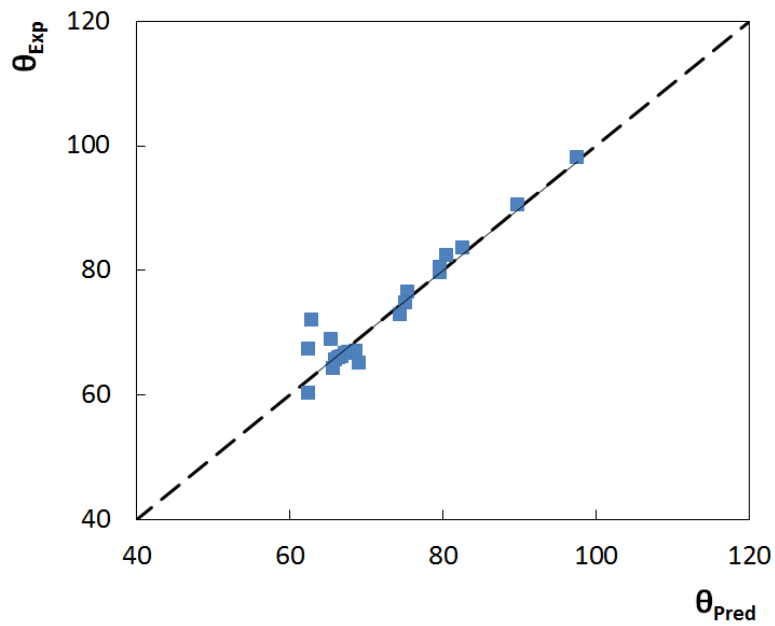


Figure S29. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S26.

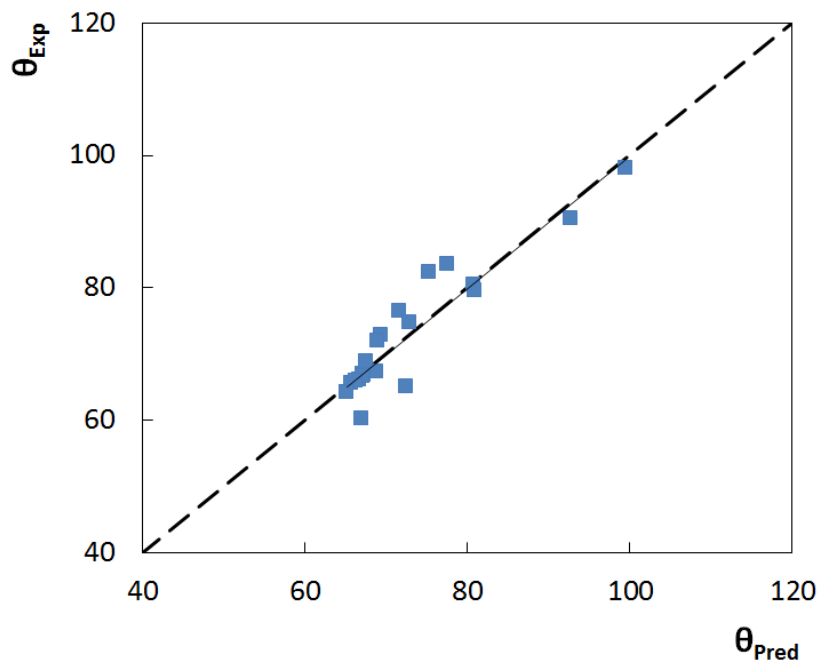


Figure S30. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S27.



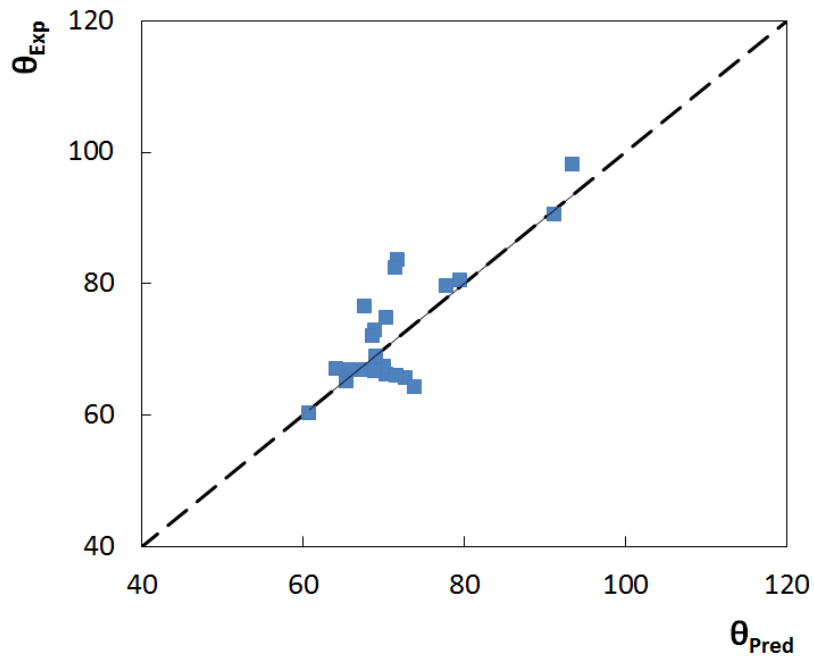


Figure S31. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S28.

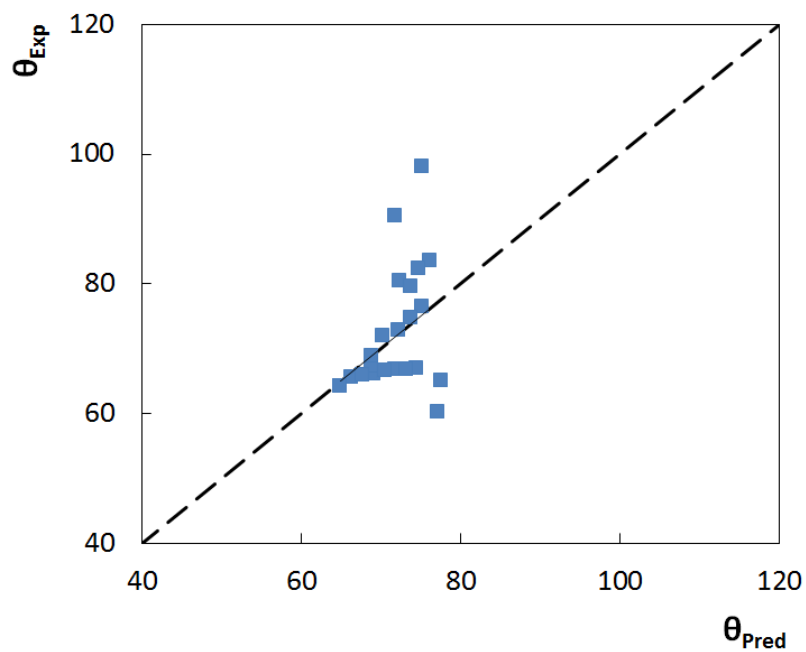


Figure S32. Comparison between experimental,  $\theta_{Exp}$ , and predictive,  $\theta_{Pred}$ , contact angles values using Equation S29.

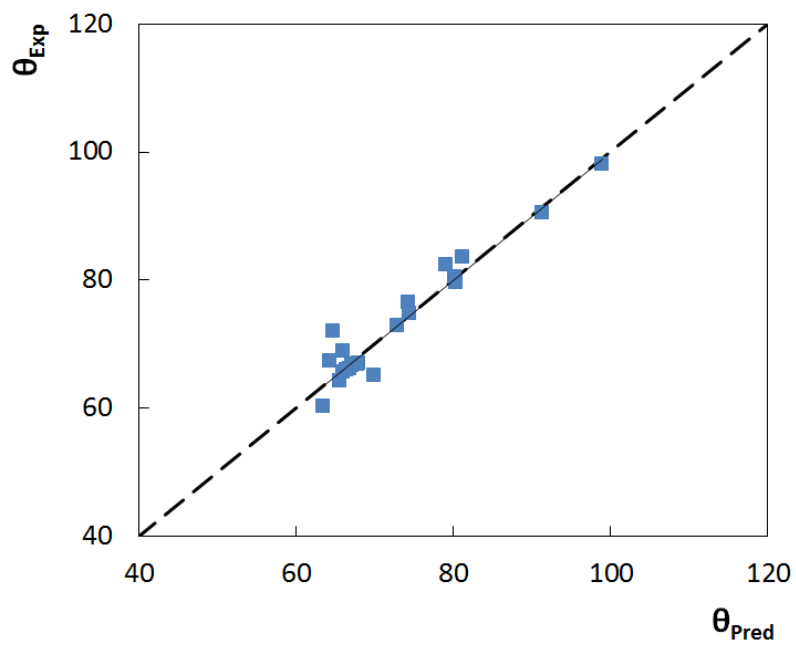


Figure S33. Comparison between experimental,  $\theta_{\text{Exp}}$ , and predictive,  $\theta_{\text{Pred}}$ , contact angles values using Equation S30.

Table S1. IL cation-anion interaction energies predicted using COSMO-RS.

Ionic Liquids	kJ·mol <sup>-1</sup>				
	$E_{\text{INT}}$	$E_{\text{MF}}$	$E_{\text{HB}}$	$E_{\text{vdW}}$	$E_{\text{Ring}}$
[C <sub>4</sub> C <sub>1</sub> im][Ac]	-39.391	55.317	-39.721	-55.532	-3.912
[C <sub>4</sub> C <sub>1</sub> im][DMP]	-41.260	53.515	-32.355	-65.029	-3.912
[C <sub>4</sub> C <sub>1</sub> im][TFA]	-38.476	37.244	-23.927	-52.666	-3.912
[C <sub>4</sub> C <sub>1</sub> im][N(CN) <sub>2</sub> ]	-40.886	36.989	-22.122	-56.721	-3.912
[C <sub>4</sub> C <sub>1</sub> im][EtSO <sub>4</sub> ]	-40.066	43.661	-21.670	-63.529	-3.912
[C <sub>4</sub> C <sub>1</sub> im][MeSO <sub>4</sub> ]	-37.650	42.266	-21.450	-59.330	-3.912
[C <sub>4</sub> C <sub>1</sub> im][CF <sub>3</sub> SO <sub>3</sub> ]	-37.509	33.815	-16.711	-55.648	-3.912
[C <sub>4</sub> C <sub>1</sub> im][SCN]	-38.888	36.096	-16.640	-59.356	-3.912
[C <sub>4</sub> C <sub>1</sub> im][C(CN) <sub>3</sub> ]	-44.027	34.931	-16.300	-63.796	-3.912
[C <sub>4</sub> C <sub>1</sub> im][NTf <sub>2</sub> ]	-37.985	33.774	-9.279	-65.077	-3.912
[C <sub>4</sub> C <sub>1</sub> im][BF <sub>4</sub> ]	-25.169	31.988	-9.543	-48.748	-3.912
[C <sub>4</sub> C <sub>1</sub> im][PF <sub>6</sub> ]	-23.218	28.069	-2.791	-49.884	-3.912
[C <sub>2</sub> C <sub>1</sub> im][NTf <sub>2</sub> ]	-34.083	30.924	-9.771	-57.538	-3.912
[C <sub>3</sub> C <sub>1</sub> im][NTf <sub>2</sub> ]	-36.090	32.325	-9.642	-60.988	-3.912
[C <sub>5</sub> C <sub>1</sub> im][NTf <sub>2</sub> ]	-40.561	34.913	-9.224	-68.777	-3.912
[C <sub>6</sub> C <sub>1</sub> im][NTf <sub>2</sub> ]	-43.162	36.017	-9.068	-72.649	-3.912
[C <sub>7</sub> C <sub>1</sub> im][NTf <sub>2</sub> ]	-45.936	37.056	-8.958	-76.543	-3.912
[C <sub>8</sub> C <sub>1</sub> im][NTf <sub>2</sub> ]	-49.070	38.084	-8.768	-80.597	-3.912
[C <sub>9</sub> C <sub>1</sub> im][NTf <sub>2</sub> ]	-51.630	38.954	-8.725	-84.397	-3.912
[C <sub>3</sub> C <sub>1</sub> pip][NTf <sub>2</sub> ]	-31.199	34.438	-4.270	-63.310	-4.694
[C <sub>4</sub> C <sub>1</sub> pip][NTf <sub>2</sub> ]	-33.697	35.662	-4.132	-67.218	-4.694
[C <sub>4</sub> -4-C <sub>1</sub> py][NTf <sub>2</sub> ]	-37.666	34.808	-7.176	-67.404	-4.694

Table S2. Correlation between experimental contact angles of ILs on the polar glass surface,  $\theta_g$ , with cation-anion interaction energies estimated using COSMO-RS along with the correlation coefficient,  $R^2$ , Fisher significance parameter,  $F$ , and average absolute relative deviation, AARD.

	$R^2$	$F$	ARD/%	Equation
$\theta_g = ((-0.8837 \pm 0.1623) \times E_{MF}) + (72.8658 \pm 6.0964)$	0.5339	29.6372	9.50	(S1)
$\theta_g = ((-0.2887 \pm 0.1382) \times E_{vdW}) + (21.3776 \pm 9.0570)$	0.1186	4.3661	11.10	(S2)
$\theta_g = ((-0.0141 \pm 39.5451) \times E_{INT}) + (0.2175 \pm 8.6678)$	-0.0415	0.0040	13.84	(S3)
$\theta_g = ((0.1165 \pm 5.7849) \times E_{Ring}) + (40.5636 \pm 23.1956)$	-0.0416	0.0004	13.86	(S4)
$\theta_g = ((-0.0070 \pm 0.1918) \times E_{MF}) + ((0.7307 \pm 0.1318) \times E_{HB}) + (50.1589 \pm 5.7775)$	0.7918	48.5403	5.30	(S5)
$\theta_g = ((0.7062 \pm 0.0771) \times E_{HB}) + ((-0.0769 \pm 0.0694) \times E_{vdW}) + (44.5813 \pm 4.9802)$	0.8024	51.7479	4.99	(S6)
$\theta_g = ((-0.9578 \pm 0.1138) \times E_{MF}) + ((-0.3636 \pm 0.0704) \times E_{vdW}) + (52.0437 \pm 5.8522)$	0.7746	43.9652	5.49	(S7)
$\theta_g = ((-0.8991 \pm 0.1653) \times E_{MF}) + ((2.8594 \pm 3.9408) \times E_{Ring}) + (84.8779 \pm 17.6632)$	0.5245	14.7895	9.39	(S8)
$\theta_g = ((-0.2895 \pm 0.1413) \times E_{vdW}) + ((0.5986 \pm 5.4392) \times E_{Ring}) + (23.7297 \pm 23.2869)$	0.0808	2.0992	11.10	(S9)
$\theta_g = ((-0.3733 \pm 0.2782) \times E_{MF}) + ((0.4561 \pm 0.2012) \times E_{HB}) + ((-0.1811 \pm 0.1034) \times E_{vdW}) + (48.3177 \pm 5.6326)$	0.8090	36.2980	4.91	(S10)

Table S3. Correlation between experimental contact angles of ILs on the polar Al-plate surface,  $\theta_{Al}$ , with cation-anion interaction energies estimated using COSMO-RS along with the correlation coefficient,  $R^2$ , Fisher significance parameter,  $F$ , average absolute relative deviation, AARD.

	$R^2$	$F$	AARD/%	Equation
$\theta_{Al} = ((-1.2595 \pm 0.1899) \times E_{MF}) + (92.1915 \pm 7.1305)$	0.6324	44.0086	9.73	(S11)
$\theta_{Al} = ((-0.3846 \pm 0.1816) \times E_{vdW}) + (20.5559 \pm 11.9039)$	0.1222	4.4831	13.83	(S12)
$\theta_{Al} = ((0.0320 \pm 0.2864) \times E_{INT}) + (46.7448 \pm 11.4138)$	-0.0415	0.0040	13.84	(S13)
$\theta_{Al} = ((-5.3405 \pm 7.5405) \times E_{Ring}) + (24.1149 \pm 30.2355)$	-0.0203	0.5016	15.47	(S14)
$\theta_{Al} = ((-0.0314 \pm 0.1453) \times E_{MF}) + ((1.0236 \pm 0.0998) \times E_{HB}) + (60.3833 \pm 4.3775)$	0.9311	169.9155	3.91	(S15)
$\theta_{Al} = ((1.0113 \pm 0.0570) \times E_{HB}) + ((-0.0813 \pm 0.0513) \times E_{vdW}) + (53.7848 \pm 3.6810)$	0.9377	189.3162	3.54	(S16)
$\theta_{Al} = ((-1.3595 \pm 0.1044) \times E_{MF}) + ((-0.4908 \pm 0.0647) \times E_{vdW}) + (64.0847 \pm 5.3706)$	0.8906	102.7360	4.60	(S17)
$\theta_{Al} = ((-1.2514 \pm 0.1951) \times E_{MF}) + ((-1.5229 \pm 4.6509) \times E_{Ring}) + (85.7937 \pm 20.8460)$	0.6182	21.2394	9.66	(S18)
$\theta_{Al} = ((-0.3793 \pm 0.1839) \times E_{vdW}) + ((-4.7088 \pm 7.0831) \times E_{Ring}) + (2.0548 \pm 30.3247)$	0.1014	2.4104	13.64	(S19)
$\theta_{Al} = ((-0.4494 \pm 0.1913) \times E_{MF}) + ((0.7103 \pm 0.1383) \times E_{HB}) + ((-0.2067 \pm 0.0711) \times E_{Ring}) + (48.3177 \pm 5.6326)$	0.8090	36.2980	4.91	(S20)

Table S4. Correlation between experimental contact angles of ILs on the nonpolar Teflon surface,  $\theta_T$ , with cation-anion interaction energies estimated using COSMO-RS along with the correlation coefficient,  $R^2$ , Fisher significance parameter,  $F$ , average absolute relative deviation, AARD.

	$R^2$	$F$	ARD/%	Equation
$\theta_T = ((1.1949 \pm 0.1842) \times E_{MF}) + (27.3679 \pm 6.9191)$	0.6216	42.0710	5.74	(S21)
$\theta_T = ((0.3592 \pm 0.1745) \times E_{vdW}) + (94.9605 \pm 11.4345)$	0.1145	4.2373	7.77	(S22)
$\theta_T = ((-0.0424 \pm 0.2738) \times E_{INT}) + (70.0134 \pm 19.9138)$	-0.0406	0.0239	10.03	(S23)
$\theta_T = ((3.3591 \pm 7.2545) \times E_{Ring}) + (85.1209 \pm 29.0887)$	-0.0324	0.2144	9.94	(S24)
$\theta_T = ((0.0393 \pm 0.1591) \times E_{MF}) + ((-0.9632 \pm 0.1093) \times E_{HB}) + (57.2996 \pm 4.7905)$	0.9097	127.0615	2.68	(S25)
$\theta_T = ((-0.9591 \pm 0.0715) \times E_{HB}) + ((0.0715 \pm 0.0572) \times E_{vdW}) + (63.4504 \pm 4.1067)$	0.9153	136.0847	2.53	(S26)
$\theta_T = ((1.2886 \pm 0.1096) \times E_{MF}) + ((0.4598 \pm 0.0678) \times E_{vdW}) + (53.7009 \pm 5.6363)$	0.8682	83.3756	2.89	(S27)
$\theta_T = ((1.1965 \pm 0.1897) \times E_{MF}) + ((-0.2912 \pm 4.5231) \times E_{Ring}) + (26.1444 \pm 20.2729)$	0.6052	20.1647	5.75	(S28)
$\theta_T = ((-0.3561 \pm 0.1777) \times E_{vdW}) + ((2.7661 \pm 6.8446) \times E_{Ring}) + (105.8287 \pm 29.3037)$	0.0826	2.1264	7.72	(S29)
$\theta_T = ((-0.4222 \pm 0.2211) \times E_{MF}) + ((-0.6762 \pm 0.1598) \times E_{HB}) + ((0.1893 \pm 0.0821) \times E_{Ring}) + (59.2244 \pm 4.4741)$	0.8090	36.2980	4.91	(S30)

Table S5. Full name, abbreviation, and numbering of IL cation and anion.

No.	Name	Abbreviations
<b>Cation</b>		
1	1,3-dimethylimidazolium	[C <sub>1</sub> C <sub>1</sub> im]
2	1-ethyl-3-methylimidazolium	[C <sub>2</sub> C <sub>1</sub> im]
3	1-propyl-3-methylimidazolium	[C <sub>3</sub> C <sub>1</sub> im]
4	1-butyl-3-methylimidazolium	[C <sub>4</sub> C <sub>1</sub> im]
5	1-pentyl-3-methylimidazolium	[C <sub>5</sub> C <sub>1</sub> im]
6	1-hexyl-3-methylimidazolium	[C <sub>6</sub> C <sub>1</sub> im]
7	1-heptyl-3-methylimidazolium	[C <sub>7</sub> C <sub>1</sub> im]
8	1-octyl-3-methylimidazolium	[C <sub>8</sub> C <sub>1</sub> im]
9	1-nonyl-3-methylimidazolium	[C <sub>9</sub> C <sub>1</sub> im]
10	1-decyl-3-methylimidazolium	[C <sub>10</sub> C <sub>1</sub> im]
<b>Anion</b>		
1	Acetate	[Ac]
2	Propionate	[Pro]
3	Butanoate	[But]
4	Pentanoate	[Pen]
5	Hexanoate	[Hex]
6	Decanoate	[Dec]
7	Trifluoroacetate	[TFA]
8	Heptafluorobutanoate	[HFBu]
9	Bis(2,4,4-trimethylpentyl)phosphinate	[Tm2P]
10	Bis(pentafluoroethyl)phosphinate	[Pf2P]
11	Dimethylphosphate	[DMP]
12	Diethylphosphate	[DEP]
13	Dibutylphosphate	[DBP]
14	Tris(pentafluoroethyl)trifluorophosphate	[eFAP]
15	Tris(nonafluorobutyl)trifluorophosphate	[bFAP]
16	Chloride	Cl
17	Bromide	Br
18	Iodide	I
19	Triiodide	[I <sub>3</sub> ]
20	Methanesulfonate	[CH <sub>3</sub> SO <sub>3</sub> ]
21	Trifluoromethanesulfonate	[CF <sub>3</sub> SO <sub>3</sub> ]
22	Perfluorobutanesulfonate	[PfbSO <sub>3</sub> ]
23	Perchlorate	[ClO <sub>4</sub> ]
24	Nitrate	[NO <sub>3</sub> ]
25	Hydrogensulfate	[HSO <sub>4</sub> ]
26	Methylsulfate	[MeSO <sub>4</sub> ]
27	Ethylsulfate	[EtSO <sub>4</sub> ]
28	Butylsulfate	[BuSO <sub>4</sub> ]
29	Octylsulfate	[OcSO <sub>4</sub> ]

30	Methoxyethylsulfate	[MeOEtSO <sub>4</sub> ]
31	Ethoxyethylsulfate	[EtOEtSO <sub>4</sub> ]
32	2-(2-methoxyethoxy)ethylsulfate	[MeOEtOSO <sub>4</sub> ]
33	Thiocyanate	[SCN]
34	Dicyanamide	[N(CN) <sub>2</sub> ]
35	Tricyanomethanide	[C(CN) <sub>3</sub> ]
36	Tetracyanoborate	[B(CN) <sub>4</sub> ]
37	Chlorotrifluoroborate	[BClF <sub>3</sub> ]
38	Tetrafluoroborate	[BF <sub>4</sub> ]
39	Tetrachloroborate	[BCl <sub>4</sub> ]
40	Hexafluorophosphate	[PF <sub>6</sub> ]
41	Hexafluoroarsenate	[AsF <sub>6</sub> ]
42	Hexafluoroantimonate	[SbF <sub>6</sub> ]
43	Bis(trifluoromethyl)imide	[BETI]
44	Bis(trifluoromethylsulfonyl)amide	[Tf <sub>2</sub> N]
45	Bis(pentafluoroethylsulfonyl)amide	[Pf <sub>2</sub> N]
46	Imidodiphosphorylfluoride	[Impf]
47	Bis(trifluoromethylsulfonyl)methide	[Tf <sub>2</sub> C]
48	Tris(trifluoromethylsulfonyl)methide	[Tf <sub>3</sub> C]

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Table S6. Cation-anion interaction energies and the predicted contact angles on the glass, Al-plate, and PTFE surfaces using Equations 3, 5, and 7, respectively.

Ionic Liquids	Interaction Energy/kJ·mol <sup>-1</sup>					Contact Angle/°		
	$E_{INT}$	$E_{MF}$	$E_{HB}$	$E_{vdW}$	$E_{Ring}$	Glass	Al-plate	PTFE
[C1C1im][Ac]	-30.85	54.94	-41.99	-43.80	-3.91	17.18	14.22	101.62
[C2C1im][Ac]	-32.20	55.42	-40.63	-47.38	-3.91	18.32	15.74	100.15
[C3C1im][Ac]	-35.24	55.29	-40.07	-51.16	-3.91	18.78	16.37	99.54
[C4C1im][Ac]	-39.39	55.32	-39.72	-55.53	-3.91	19.07	16.76	99.17
[C5C1im][Ac]	-43.09	55.21	-39.67	-59.42	-3.91	19.12	16.82	99.11
[C6C1im][Ac]	-46.82	55.38	-39.44	-63.52	-3.91	19.31	17.08	98.86
[C7C1im][Ac]	-50.81	55.56	-39.55	-67.57	-3.91	19.21	16.95	98.99
[C8C1im][Ac]	-54.65	55.96	-39.18	-71.82	-3.91	19.53	17.37	98.58
[C9C1im][Ac]	-57.67	56.22	-39.19	-75.74	-3.91	19.52	17.36	98.59
[C10C1im][Ac]	-61.50	56.86	-38.72	-80.03	-3.91	19.91	17.89	98.08
[C1C1im][Pro]	-36.64	52.53	-41.48	-47.69	-3.91	17.61	14.80	101.06
[C2C1im][Pro]	-37.68	53.41	-40.19	-51.31	-3.91	18.68	16.23	99.67
[C3C1im][Pro]	-40.51	53.59	-39.70	-55.11	-3.91	19.09	16.79	99.14
[C4C1im][Pro]	-44.43	53.87	-39.38	-59.49	-3.91	19.36	17.15	98.79
[C5C1im][Pro]	-48.01	53.93	-39.35	-63.38	-3.91	19.38	17.17	98.77
[C6C1im][Pro]	-51.63	54.23	-39.14	-67.48	-3.91	19.56	17.41	98.54
[C7C1im][Pro]	-55.56	54.50	-39.27	-71.55	-3.91	19.45	17.26	98.68
[C8C1im][Pro]	-59.36	54.96	-38.92	-75.79	-3.91	19.74	17.66	98.30
[C9C1im][Pro]	-62.35	55.28	-38.93	-79.73	-3.91	19.73	17.65	98.31
[C10C1im][Pro]	-66.16	55.93	-38.48	-84.01	-3.91	20.11	18.16	97.82
[C1C1im][But]	-40.53	52.52	-41.36	-51.68	-3.91	17.70	14.92	100.94
[C2C1im][But]	-41.43	53.57	-40.10	-55.33	-3.91	18.76	16.34	99.57

[C3C1im][But]	-44.17	53.89	-39.63	-59.14	-3.91	19.15	16.87	99.06
[C4C1im][But]	-48.00	54.28	-39.32	-63.53	-3.91	19.41	17.21	98.73
[C5C1im][But]	-51.55	54.41	-39.31	-67.44	-3.91	19.41	17.22	98.73
[C6C1im][But]	-55.14	54.76	-39.11	-71.55	-3.91	19.58	17.45	98.51
[C7C1im][But]	-59.06	55.05	-39.26	-75.62	-3.91	19.46	17.28	98.66
[C8C1im][But]	-62.85	55.53	-38.91	-79.87	-3.91	19.75	17.67	98.29
[C9C1im][But]	-65.83	55.87	-38.92	-83.81	-3.91	19.74	17.65	98.31
[C10C1im][But]	-69.64	56.52	-38.47	-88.09	-3.91	20.11	18.16	97.82
[C1C1im][Pen]	-44.29	52.64	-41.18	-55.75	-3.91	17.85	15.12	100.74
[C2C1im][Pen]	-45.13	53.79	-39.93	-59.42	-3.91	18.90	16.53	99.39
[C3C1im][Pen]	-47.82	54.18	-39.48	-63.24	-3.91	19.28	17.04	98.90
[C4C1im][Pen]	-51.59	54.65	-39.18	-67.64	-3.91	19.52	17.37	98.58
[C5C1im][Pen]	-55.11	54.83	-39.18	-71.56	-3.91	19.52	17.37	98.58
[C6C1im][Pen]	-58.68	55.21	-38.99	-75.67	-3.91	19.68	17.58	98.38
[C7C1im][Pen]	-62.59	55.53	-39.14	-79.74	-3.91	19.56	17.41	98.54
[C8C1im][Pen]	-66.37	56.02	-38.80	-83.99	-3.91	19.84	17.79	98.17
[C9C1im][Pen]	-69.36	56.36	-38.82	-87.94	-3.91	19.83	17.77	98.19
[C10C1im][Pen]	-73.17	57.03	-38.38	-92.22	-3.91	20.20	18.27	97.72
[C1C1im][Hex]	-47.90	52.89	-41.03	-59.76	-3.91	17.98	15.30	100.58
[C2C1im][Hex]	-48.71	54.07	-39.77	-63.45	-3.91	19.03	16.70	99.22
[C3C1im][Hex]	-51.40	54.51	-39.34	-67.28	-3.91	19.39	17.19	98.75
[C4C1im][Hex]	-55.12	55.03	-39.05	-71.69	-3.91	19.63	17.51	98.44
[C5C1im][Hex]	-58.63	55.24	-39.06	-75.61	-3.91	19.62	17.50	98.46
[C6C1im][Hex]	-62.18	55.65	-38.87	-79.72	-3.91	19.78	17.71	98.25
[C7C1im][Hex]	-66.10	55.97	-39.03	-83.80	-3.91	19.65	17.54	98.42
[C8C1im][Hex]	-69.87	56.48	-38.69	-88.05	-3.91	19.93	17.91	98.06
[C9C1im][Hex]	-72.87	56.82	-38.72	-92.00	-3.91	19.91	17.88	98.09
[C10C1im][Hex]	-76.69	57.48	-38.28	-96.29	-3.91	20.27	18.37	97.62

[C1C1im][Dec]	-61.96	54.26	-40.08	-76.13	-3.91	18.78	16.36	99.55
[C2C1im][Dec]	-62.79	55.44	-38.83	-79.85	-3.91	19.81	17.75	98.21
[C3C1im][Dec]	-65.49	55.93	-38.43	-83.71	-3.91	20.15	18.20	97.78
[C4C1im][Dec]	-69.13	56.54	-38.16	-88.13	-3.91	20.37	18.51	97.48
[C5C1im][Dec]	-72.66	56.80	-38.20	-92.06	-3.91	20.35	18.47	97.52
[C6C1im][Dec]	-76.21	57.23	-38.02	-96.19	-3.91	20.49	18.66	97.33
[C7C1im][Dec]	-80.13	57.57	-38.19	-100.28	-3.91	20.35	18.47	97.52
[C8C1im][Dec]	-83.90	58.09	-37.87	-104.53	-3.91	20.61	18.83	97.17
[C9C1im][Dec]	-86.93	58.44	-37.91	-108.49	-3.91	20.59	18.80	97.21
[C10C1im][Dec]	-90.75	59.09	-37.48	-112.78	-3.91	20.94	19.27	96.75
[C1C1im][TFA]	-34.32	32.49	-25.61	-41.20	-3.91	30.84	32.57	83.94
[C2C1im][TFA]	-33.83	34.74	-24.54	-44.68	-3.91	31.73	33.76	82.79
[C3C1im][TFA]	-35.92	35.96	-24.32	-48.36	-3.91	31.91	34.01	82.55
[C4C1im][TFA]	-38.48	37.24	-23.93	-52.67	-3.91	32.24	34.45	82.13
[C5C1im][TFA]	-41.37	38.07	-23.93	-56.50	-3.91	32.23	34.44	82.13
[C6C1im][TFA]	-44.30	39.02	-23.74	-60.54	-3.91	32.40	34.66	81.93
[C7C1im][TFA]	-47.49	39.88	-23.75	-64.57	-3.91	32.38	34.65	81.94
[C8C1im][TFA]	-50.82	40.82	-23.47	-68.76	-3.91	32.62	34.96	81.64
[C9C1im][TFA]	-53.44	41.56	-23.46	-72.66	-3.91	32.63	34.98	81.62
[C10C1im][TFA]	-56.85	42.53	-23.07	-76.90	-3.91	32.95	35.41	81.20
[C1C1im][HFBu]	-36.11	34.08	-23.70	-47.57	-3.91	32.43	34.71	81.88
[C2C1im][HFBu]	-36.03	35.77	-22.70	-50.92	-3.91	33.27	35.83	80.80
[C3C1im][HFBu]	-38.27	36.82	-22.53	-54.47	-3.91	33.40	36.02	80.62
[C4C1im][HFBu]	-40.77	38.00	-22.16	-58.64	-3.91	33.72	36.44	80.22
[C5C1im][HFBu]	-43.70	38.77	-22.18	-62.38	-3.91	33.69	36.41	80.25
[C6C1im][HFBu]	-46.61	39.62	-22.00	-66.32	-3.91	33.84	36.61	80.05
[C7C1im][HFBu]	-49.83	40.39	-22.02	-70.26	-3.91	33.83	36.59	80.07
[C8C1im][HFBu]	-53.18	41.23	-21.77	-74.36	-3.91	34.04	36.87	79.80

[C9C1im][HFBu]	-55.85	41.89	-21.75	-78.20	-3.91	34.06	36.89	79.78
[C10C1im][HFBu]	-59.27	42.75	-21.39	-82.36	-3.91	34.36	37.30	79.39
[C1C1im][Tm2P]	-85.11	52.45	-39.76	-97.80	-3.91	19.04	16.72	99.21
[C2C1im][Tm2P]	-86.27	53.32	-38.56	-101.53	-3.91	20.04	18.07	97.91
[C3C1im][Tm2P]	-89.15	53.73	-38.20	-105.40	-3.91	20.35	18.47	97.52
[C4C1im][Tm2P]	-92.79	54.30	-37.93	-109.82	-3.91	20.57	18.77	97.23
[C5C1im][Tm2P]	-96.40	54.56	-38.01	-113.77	-3.91	20.50	18.67	97.32
[C6C1im][Tm2P]	-99.95	55.00	-37.85	-117.89	-3.91	20.63	18.86	97.15
[C7C1im][Tm2P]	-103.94	55.32	-38.05	-121.99	-3.91	20.47	18.64	97.36
[C8C1im][Tm2P]	-107.72	55.82	-37.74	-126.24	-3.91	20.72	18.98	97.03
[C9C1im][Tm2P]	-110.80	56.17	-37.77	-130.21	-3.91	20.70	18.94	97.06
[C10C1im][Tm2P]	-114.67	56.76	-37.38	-134.49	-3.91	21.03	19.38	96.64
[C1C1im][Pf2P]	-37.06	32.53	-18.07	-52.84	-3.91	37.12	41.01	75.81
[C2C1im][Pf2P]	-37.51	33.61	-17.20	-56.08	-3.91	37.85	41.99	74.87
[C3C1im][Pf2P]	-39.99	34.52	-17.11	-59.53	-3.91	37.93	42.09	74.77
[C4C1im][Pf2P]	-42.37	35.60	-16.74	-63.60	-3.91	38.23	42.50	74.38
[C5C1im][Pf2P]	-45.30	36.38	-16.77	-67.28	-3.91	38.21	42.47	74.41
[C6C1im][Pf2P]	-48.17	37.21	-16.61	-71.13	-3.91	38.34	42.65	74.23
[C7C1im][Pf2P]	-51.32	37.95	-16.59	-75.00	-3.91	38.35	42.67	74.22
[C8C1im][Pf2P]	-54.66	38.76	-16.38	-79.03	-3.91	38.53	42.91	73.99
[C9C1im][Pf2P]	-57.36	39.41	-16.35	-82.82	-3.91	38.56	42.94	73.95
[C10C1im][Pf2P]	-60.78	40.17	-16.03	-86.91	-3.91	38.82	43.29	73.61
[C1C1im][DMP]	-35.15	50.96	-34.82	-53.25	-3.91	23.16	22.26	93.88
[C2C1im][DMP]	-35.20	52.50	-33.27	-56.86	-3.91	24.45	23.98	92.21
[C3C1im][DMP]	-37.78	52.98	-32.80	-60.65	-3.91	24.84	24.51	91.70
[C4C1im][DMP]	-41.26	53.52	-32.35	-65.03	-3.91	25.21	25.01	91.22
[C5C1im][DMP]	-44.69	53.73	-32.30	-68.92	-3.91	25.26	25.08	91.16
[C6C1im][DMP]	-48.16	54.17	-32.08	-73.02	-3.91	25.44	25.32	90.93

[C7C1im][DMP]	-51.79	54.63	-32.10	-77.08	-3.91	25.43	25.30	90.94
[C8C1im][DMP]	-55.44	55.24	-31.74	-81.32	-3.91	25.72	25.70	90.56
[C9C1im][DMP]	-58.35	55.65	-31.76	-85.25	-3.91	25.71	25.68	90.57
[C10C1im][DMP]	-61.93	56.46	-31.26	-89.53	-3.91	26.13	26.24	90.04
[C1C1im][DEP]	-44.23	51.48	-35.16	-61.56	-3.91	22.88	21.88	94.24
[C2C1im][DEP]	-44.07	53.26	-33.62	-65.21	-3.91	24.16	23.59	92.59
[C3C1im][DEP]	-46.53	53.94	-33.19	-69.03	-3.91	24.52	24.08	92.12
[C4C1im][DEP]	-49.86	54.66	-32.77	-73.42	-3.91	24.87	24.55	91.67
[C5C1im][DEP]	-53.23	54.98	-32.74	-77.33	-3.91	24.89	24.58	91.63
[C6C1im][DEP]	-56.66	55.49	-32.54	-81.44	-3.91	25.06	24.81	91.42
[C7C1im][DEP]	-60.27	56.00	-32.57	-85.51	-3.91	25.03	24.77	91.45
[C8C1im][DEP]	-63.91	56.63	-32.23	-89.76	-3.91	25.32	25.15	91.09
[C9C1im][DEP]	-66.84	57.06	-32.25	-93.69	-3.91	25.30	25.12	91.11
[C10C1im][DEP]	-70.43	57.86	-31.76	-97.98	-3.91	25.71	25.67	90.58
[C1C1im][DBP]	-57.54	52.99	-34.20	-77.75	-3.91	23.68	22.95	93.21
[C2C1im][DBP]	-57.47	54.74	-32.71	-81.45	-3.91	24.92	24.61	91.61
[C3C1im][DBP]	-59.98	55.49	-32.35	-85.29	-3.91	25.22	25.02	91.21
[C4C1im][DBP]	-63.23	56.30	-31.95	-89.70	-3.91	25.55	25.46	90.79
[C5C1im][DBP]	-66.62	56.70	-31.96	-93.63	-3.91	25.54	25.45	90.80
[C6C1im][DBP]	-70.03	57.25	-31.78	-97.75	-3.91	25.69	25.65	90.60
[C7C1im][DBP]	-73.69	57.76	-31.85	-101.84	-3.91	25.64	25.58	90.67
[C8C1im][DBP]	-77.34	58.39	-31.53	-106.09	-3.91	25.90	25.94	90.33
[C9C1im][DBP]	-80.33	58.81	-31.57	-110.04	-3.91	25.87	25.90	90.37
[C10C1im][DBP]	-83.95	59.59	-31.10	-114.33	-3.91	26.26	26.42	89.87
[C1C1im][eFAP]	-21.90	35.51	-0.73	-56.72	-3.91	51.58	60.43	57.10
[C2C1im][eFAP]	-23.95	35.24	-0.66	-59.84	-3.91	51.63	60.51	57.03
[C3C1im][eFAP]	-26.94	35.87	-0.66	-63.19	-3.91	51.64	60.52	57.02
[C4C1im][eFAP]	-29.59	36.54	-0.62	-67.13	-3.91	51.67	60.55	56.99

[C5C1im][eFAP]	-32.60	37.37	-0.62	-70.75	-3.91	51.67	60.56	56.98
[C6C1im][eFAP]	-35.62	38.07	-0.60	-74.51	-3.91	51.68	60.58	56.97
[C7C1im][eFAP]	-38.78	38.75	-0.59	-78.32	-3.91	51.69	60.59	56.95
[C8C1im][eFAP]	-42.31	39.41	-0.58	-82.26	-3.91	51.70	60.61	56.94
[C9C1im][eFAP]	-45.25	40.04	-0.57	-86.01	-3.91	51.71	60.61	56.93
[C10C1im][eFAP]	-48.93	40.52	-0.55	-90.01	-3.91	51.73	60.64	56.91
[C1C1im][bFAP]	-37.36	40.73	-0.77	-77.33	-3.91	51.55	60.39	57.14
[C2C1im][bFAP]	-39.75	40.00	-0.70	-80.33	-3.91	51.60	60.47	57.07
[C3C1im][bFAP]	-43.02	40.20	-0.70	-83.55	-3.91	51.60	60.47	57.07
[C4C1im][bFAP]	-45.86	40.51	-0.67	-87.30	-3.91	51.63	60.51	57.03
[C5C1im][bFAP]	-49.00	41.05	-0.66	-90.76	-3.91	51.63	60.51	57.03
[C6C1im][bFAP]	-52.10	41.50	-0.65	-94.36	-3.91	51.64	60.52	57.02
[C7C1im][bFAP]	-55.34	41.93	-0.64	-98.00	-3.91	51.65	60.53	57.01
[C8C1im][bFAP]	-58.90	42.39	-0.63	-101.78	-3.91	51.66	60.55	56.99
[C9C1im][bFAP]	-61.89	42.83	-0.62	-105.37	-3.91	51.67	60.56	56.99
[C10C1im][bFAP]	-65.58	43.13	-0.60	-109.21	-3.91	51.68	60.58	56.96
[C1C1im]Cl	-14.65	60.18	-32.97	-41.86	-3.91	24.70	24.33	91.88
[C2C1im]Cl	-17.20	59.25	-31.45	-45.39	-3.91	25.97	26.02	90.25
[C3C1im]Cl	-21.13	58.14	-30.84	-49.13	-3.91	26.48	26.71	89.59
[C4C1im]Cl	-25.87	57.39	-30.34	-53.49	-3.91	26.89	27.27	89.05
[C5C1im]Cl	-29.97	56.78	-30.17	-57.38	-3.91	27.04	27.46	88.86
[C6C1im]Cl	-33.99	56.60	-29.90	-61.46	-3.91	27.26	27.76	88.58
[C7C1im]Cl	-38.02	56.57	-29.85	-65.52	-3.91	27.30	27.82	88.52
[C8C1im]Cl	-42.01	56.80	-29.46	-69.76	-3.91	27.63	28.25	88.10
[C9C1im]Cl	-45.16	56.90	-29.45	-73.67	-3.91	27.64	28.27	88.08
[C10C1im]Cl	-48.97	57.52	-28.95	-77.96	-3.91	28.05	28.83	87.54
[C1C1im]Br	-20.01	52.66	-27.75	-44.91	-3.91	29.05	30.17	86.26
[C2C1im]Br	-21.83	52.36	-26.30	-48.36	-3.91	30.26	31.80	84.68

[C3C1im]Br	-25.47	51.60	-25.77	-52.04	-3.91	30.71	32.39	84.11
[C4C1im]Br	-29.71	51.25	-25.22	-56.43	-3.91	31.16	33.01	83.52
[C5C1im]Br	-33.56	50.91	-25.04	-60.31	-3.91	31.31	33.20	83.33
[C6C1im]Br	-37.28	51.01	-24.77	-64.37	-3.91	31.54	33.51	83.03
[C7C1im]Br	-40.97	51.24	-24.66	-68.41	-3.91	31.63	33.63	82.92
[C8C1im]Br	-44.76	51.69	-24.29	-72.65	-3.91	31.94	34.05	82.51
[C9C1im]Br	-47.70	51.99	-24.25	-76.53	-3.91	31.97	34.09	82.48
[C10C1im]Br	-51.32	52.77	-23.77	-80.82	-3.91	32.37	34.63	81.95
[C1C1im]I	-29.89	42.55	-22.05	-50.39	-3.91	33.80	36.55	80.10
[C2C1im]I	-30.59	43.27	-20.63	-53.81	-3.91	34.98	38.14	78.57
[C3C1im]I	-33.65	43.20	-20.18	-57.46	-3.91	35.36	38.65	78.09
[C4C1im]I	-37.09	43.52	-19.61	-61.82	-3.91	35.84	39.29	77.47
[C5C1im]I	-40.46	43.69	-19.44	-65.69	-3.91	35.98	39.48	77.28
[C6C1im]I	-43.74	44.22	-19.16	-69.74	-3.91	36.21	39.79	76.99
[C7C1im]I	-46.98	44.85	-19.00	-73.78	-3.91	36.34	39.97	76.82
[C8C1im]I	-50.45	45.63	-18.66	-78.00	-3.91	36.63	40.35	76.45
[C9C1im]I	-53.13	46.22	-18.60	-81.89	-3.91	36.68	40.41	76.39
[C10C1im]I	-56.49	47.23	-18.15	-86.16	-3.91	37.05	40.92	75.90
[C1C1im][I3]	-59.86	23.55	-3.47	-79.94	-3.91	49.29	57.37	60.06
[C2C1im][I3]	-59.46	25.49	-3.12	-83.01	-3.91	49.58	57.76	59.68
[C3C1im][I3]	-60.75	27.66	-3.05	-86.33	-3.91	49.64	57.83	59.61
[C4C1im][I3]	-62.18	29.64	-2.89	-90.40	-3.91	49.77	58.01	59.44
[C5C1im][I3]	-64.33	31.32	-2.85	-94.11	-3.91	49.81	58.06	59.39
[C6C1im][I3]	-66.62	32.81	-2.78	-97.99	-3.91	49.87	58.14	59.31
[C7C1im][I3]	-69.14	34.18	-2.71	-101.90	-3.91	49.92	58.21	59.24
[C8C1im][I3]	-72.14	35.47	-2.63	-105.98	-3.91	49.99	58.30	59.16
[C9C1im][I3]	-74.55	36.61	-2.60	-109.80	-3.91	50.01	58.34	59.13
[C10C1im][I3]	-77.77	37.67	-2.50	-113.93	-3.91	50.10	58.45	59.01

[C1C1im][CH3SO3]	-27.92	49.52	-31.26	-46.18	-3.91	26.13	26.24	90.03
[C2C1im][CH3SO3]	-28.24	50.64	-29.62	-49.76	-3.91	27.49	28.07	88.27
[C3C1im][CH3SO3]	-31.12	50.78	-29.11	-53.54	-3.91	27.92	28.64	87.72
[C4C1im][CH3SO3]	-34.71	51.10	-28.58	-57.91	-3.91	28.36	29.24	87.15
[C5C1im][CH3SO3]	-38.19	51.19	-28.46	-61.80	-3.91	28.46	29.37	87.02
[C6C1im][CH3SO3]	-41.65	51.59	-28.20	-65.90	-3.91	28.68	29.66	86.74
[C7C1im][CH3SO3]	-45.19	52.05	-28.14	-69.96	-3.91	28.73	29.74	86.67
[C8C1im][CH3SO3]	-48.79	52.68	-27.76	-74.20	-3.91	29.05	30.16	86.26
[C9C1im][CH3SO3]	-51.65	53.12	-27.74	-78.13	-3.91	29.06	30.18	86.25
[C10C1im][CH3SO3]	-55.15	54.00	-27.23	-82.42	-3.91	29.49	30.75	85.69
[C1C1im][CF3SO3]	-34.78	28.10	-18.62	-44.26	-3.91	36.67	40.40	76.40
[C2C1im][CF3SO3]	-33.69	30.66	-17.43	-47.72	-3.91	37.66	41.73	75.11
[C3C1im][CF3SO3]	-35.50	32.22	-17.19	-51.38	-3.91	37.86	42.00	74.86
[C4C1im][CF3SO3]	-37.51	33.82	-16.71	-55.65	-3.91	38.26	42.54	74.34
[C5C1im][CF3SO3]	-40.12	34.91	-16.64	-59.47	-3.91	38.31	42.61	74.27
[C6C1im][CF3SO3]	-42.79	36.05	-16.43	-63.48	-3.91	38.49	42.85	74.04
[C7C1im][CF3SO3]	-45.63	37.13	-16.32	-67.49	-3.91	38.58	42.98	73.92
[C8C1im][CF3SO3]	-48.76	38.24	-16.04	-71.67	-3.91	38.82	43.29	73.62
[C9C1im][CF3SO3]	-51.28	39.11	-15.99	-75.56	-3.91	38.85	43.34	73.57
[C10C1im][CF3SO3]	-54.47	40.20	-15.60	-79.78	-3.91	39.18	43.78	73.14
[C1C1im][PfbSO3]	-37.44	33.08	-16.68	-53.84	-3.91	38.28	42.57	74.30
[C2C1im][PfbSO3]	-37.09	34.76	-15.61	-57.10	-3.91	39.17	43.77	73.15
[C3C1im][PfbSO3]	-39.24	35.92	-15.44	-60.58	-3.91	39.32	43.96	72.97
[C4C1im][PfbSO3]	-41.37	37.20	-15.01	-64.66	-3.91	39.67	44.44	72.51
[C5C1im][PfbSO3]	-44.12	38.10	-14.98	-68.34	-3.91	39.70	44.47	72.48
[C6C1im][PfbSO3]	-46.87	39.04	-14.80	-72.21	-3.91	39.85	44.68	72.28
[C7C1im][PfbSO3]	-49.81	39.92	-14.71	-76.09	-3.91	39.92	44.78	72.18
[C8C1im][PfbSO3]	-53.02	40.84	-14.47	-80.14	-3.91	40.12	45.05	71.92



[C9C1im][PfbSO3]	-55.64	41.57	-14.44	-83.93	-3.91	40.15	45.08	71.89
[C10C1im][PfbSO3]	-58.89	42.47	-14.08	-88.03	-3.91	40.45	45.48	71.51
[C1C1im][ClO4]	-32.89	22.95	-14.84	-41.00	-3.91	39.81	44.63	72.33
[C2C1im][ClO4]	-31.34	25.99	-13.61	-44.57	-3.91	40.84	46.01	71.00
[C3C1im][ClO4]	-32.98	27.77	-13.31	-48.32	-3.91	41.09	46.35	70.67
[C4C1im][ClO4]	-34.72	29.65	-12.79	-52.69	-3.91	41.53	46.93	70.11
[C5C1im][ClO4]	-37.07	31.01	-12.65	-56.58	-3.91	41.64	47.08	69.96
[C6C1im][ClO4]	-39.50	32.44	-12.42	-60.67	-3.91	41.84	47.35	69.71
[C7C1im][ClO4]	-42.04	33.82	-12.24	-64.74	-3.91	41.98	47.54	69.52
[C8C1im][ClO4]	-44.98	35.19	-11.96	-68.98	-3.91	42.21	47.86	69.22
[C9C1im][ClO4]	-47.29	36.32	-11.89	-72.91	-3.91	42.27	47.93	69.15
[C10C1im][ClO4]	-50.31	37.63	-11.52	-77.20	-3.91	42.58	48.35	68.74
[C1C1im][NO3]	-28.67	37.13	-26.37	-39.42	-3.91	30.20	31.71	84.77
[C2C1im][NO3]	-28.63	38.47	-24.84	-42.84	-3.91	31.48	33.43	83.11
[C3C1im][NO3]	-31.16	38.91	-24.36	-46.49	-3.91	31.88	33.96	82.60
[C4C1im][NO3]	-34.14	39.62	-23.78	-50.79	-3.91	32.36	34.62	81.97
[C5C1im][NO3]	-37.20	40.08	-23.64	-54.61	-3.91	32.48	34.77	81.82
[C6C1im][NO3]	-40.26	40.81	-23.36	-58.65	-3.91	32.71	35.08	81.52
[C7C1im][NO3]	-43.39	41.59	-23.25	-62.67	-3.91	32.81	35.22	81.39
[C8C1im][NO3]	-46.71	42.49	-22.88	-66.88	-3.91	33.11	35.62	81.00
[C9C1im][NO3]	-49.30	43.18	-22.84	-70.77	-3.91	33.15	35.67	80.95
[C10C1im][NO3]	-52.57	44.23	-22.35	-75.03	-3.91	33.55	36.22	80.43
[C1C1im][HSO4]	-61.00	34.43	-52.34	-43.09	-3.91	8.55	2.62	112.78
[C2C1im][HSO4]	-60.76	36.11	-50.88	-46.63	-3.91	9.77	4.26	111.21
[C3C1im][HSO4]	-63.20	36.79	-50.43	-50.37	-3.91	10.15	4.77	110.72
[C4C1im][HSO4]	-65.92	37.74	-49.80	-54.74	-3.91	10.67	5.47	110.04
[C5C1im][HSO4]	-68.82	38.37	-49.61	-58.61	-3.91	10.83	5.69	109.83
[C6C1im][HSO4]	-71.75	39.25	-49.29	-62.71	-3.91	11.10	6.05	109.48

[C7C1im][HSO4]	-74.72	40.15	-49.09	-66.77	-3.91	11.26	6.26	109.28
[C8C1im][HSO4]	-77.95	41.16	-48.69	-71.03	-3.91	11.59	6.71	108.85
[C9C1im][HSO4]	-80.45	41.94	-48.60	-74.95	-3.91	11.67	6.82	108.74
[C10C1im][HSO4]	-83.65	43.06	-48.09	-79.24	-3.91	12.10	7.39	108.19
[C1C1im][MeSO4]	-33.08	38.40	-23.87	-47.61	-3.91	32.29	34.52	82.07
[C2C1im][MeSO4]	-32.50	40.43	-22.38	-51.19	-3.91	33.53	36.18	80.46
[C3C1im][MeSO4]	-34.88	41.27	-22.00	-54.96	-3.91	33.85	36.61	80.05
[C4C1im][MeSO4]	-37.65	42.27	-21.45	-59.33	-3.91	34.30	37.23	79.46
[C5C1im][MeSO4]	-40.69	42.87	-21.34	-63.22	-3.91	34.39	37.35	79.34
[C6C1im][MeSO4]	-43.74	43.69	-21.10	-67.31	-3.91	34.60	37.62	79.07
[C7C1im][MeSO4]	-46.85	44.54	-20.98	-71.37	-3.91	34.70	37.76	78.94
[C8C1im][MeSO4]	-50.18	45.47	-20.64	-75.61	-3.91	34.98	38.13	78.58
[C9C1im][MeSO4]	-52.81	46.19	-20.61	-79.53	-3.91	35.00	38.17	78.55
[C10C1im][MeSO4]	-56.09	47.26	-20.14	-83.82	-3.91	35.40	38.69	78.04
[C1C1im][EtSO4]	-35.70	39.45	-24.01	-51.75	-3.91	32.17	34.36	82.22
[C2C1im][EtSO4]	-35.02	41.63	-22.55	-55.36	-3.91	33.39	36.00	80.64
[C3C1im][EtSO4]	-37.34	42.59	-22.19	-59.15	-3.91	33.69	36.40	80.26
[C4C1im][EtSO4]	-40.07	43.66	-21.67	-63.53	-3.91	34.12	36.98	79.69
[C5C1im][EtSO4]	-43.12	44.30	-21.58	-67.43	-3.91	34.20	37.08	79.60
[C6C1im][EtSO4]	-46.20	45.11	-21.35	-71.52	-3.91	34.39	37.34	79.35
[C7C1im][EtSO4]	-49.35	45.93	-21.24	-75.59	-3.91	34.48	37.46	79.23
[C8C1im][EtSO4]	-52.72	46.83	-20.92	-79.83	-3.91	34.75	37.82	78.88
[C9C1im][EtSO4]	-55.41	47.52	-20.89	-83.76	-3.91	34.77	37.85	78.85
[C10C1im][EtSO4]	-58.73	48.55	-20.43	-88.05	-3.91	35.16	38.37	78.35
[C1C1im][BuSO4]	-42.06	40.59	-23.39	-59.67	-3.91	32.69	35.06	81.54
[C2C1im][BuSO4]	-41.42	42.81	-21.99	-63.33	-3.91	33.86	36.62	80.04
[C3C1im][BuSO4]	-43.72	43.89	-21.69	-67.14	-3.91	34.11	36.96	79.71
[C4C1im][BuSO4]	-46.40	45.05	-21.20	-71.54	-3.91	34.51	37.51	79.19

[C5C1im][BuSO4]	-49.47	45.74	-21.14	-75.45	-3.91	34.56	37.57	79.12
[C6C1im][BuSO4]	-52.56	46.56	-20.93	-79.56	-3.91	34.74	37.81	78.90
[C7C1im][BuSO4]	-55.77	47.37	-20.85	-83.64	-3.91	34.81	37.90	78.80
[C8C1im][BuSO4]	-59.17	48.25	-20.54	-87.88	-3.91	35.06	38.24	78.48
[C9C1im][BuSO4]	-61.93	48.91	-20.53	-91.83	-3.91	35.07	38.26	78.46
[C10C1im][BuSO4]	-65.29	49.90	-20.09	-96.11	-3.91	35.44	38.75	77.99
[C1C1im][OcSO4]	-53.25	44.21	-22.41	-76.02	-3.91	33.50	36.15	80.49
[C2C1im][OcSO4]	-52.97	46.15	-21.09	-79.71	-3.91	34.60	37.63	79.07
[C3C1im][OcSO4]	-55.47	47.16	-20.85	-83.55	-3.91	34.80	37.89	78.81
[C4C1im][OcSO4]	-58.22	48.26	-20.41	-87.96	-3.91	35.17	38.39	78.34
[C5C1im][OcSO4]	-61.41	48.92	-20.40	-91.90	-3.91	35.18	38.41	78.32
[C6C1im][OcSO4]	-64.60	49.68	-20.22	-96.01	-3.91	35.33	38.60	78.13
[C7C1im][OcSO4]	-67.92	50.43	-20.17	-100.11	-3.91	35.38	38.67	78.07
[C8C1im][OcSO4]	-71.42	51.23	-19.90	-104.36	-3.91	35.60	38.97	77.78
[C9C1im][OcSO4]	-74.29	51.83	-19.90	-108.31	-3.91	35.60	38.97	77.78
[C10C1im][OcSO4]	-79.44	52.09	-19.93	-113.15	-3.91	35.57	38.93	77.82
[C1C1im][MeOEtSO4]	-34.97	43.15	-23.66	-57.22	-3.91	32.46	34.75	81.84
[C2C1im][MeOEtSO4]	-34.21	45.39	-22.18	-60.85	-3.91	33.69	36.40	80.25
[C3C1im][MeOEtSO4]	-36.55	46.38	-21.85	-64.64	-3.91	33.97	36.78	79.89
[C4C1im][MeOEtSO4]	-39.31	47.44	-21.33	-69.03	-3.91	34.40	37.36	79.33
[C5C1im][MeOEtSO4]	-42.40	48.07	-21.26	-72.94	-3.91	34.46	37.44	79.25
[C6C1im][MeOEtSO4]	-45.52	48.87	-21.05	-77.04	-3.91	34.64	37.68	79.02
[C7C1im][MeOEtSO4]	-48.68	49.70	-20.95	-81.11	-3.91	34.73	37.79	78.91
[C8C1im][MeOEtSO4]	-52.06	50.59	-20.63	-85.36	-3.91	34.99	38.14	78.57
[C9C1im][MeOEtSO4]	-54.76	51.29	-20.62	-89.29	-3.91	35.00	38.16	78.56
[C10C1im][MeOEtSO4]	-58.08	52.32	-20.16	-93.57	-3.91	35.38	38.67	78.07
[C1C1im][EtOEtSO4]	-38.36	43.51	-23.42	-61.45	-3.91	32.66	35.02	81.58
[C2C1im][EtOEtSO4]	-37.60	45.75	-21.96	-65.09	-3.91	33.88	36.65	80.01

[C3C1im][EtOEtSO4]	-39.88	46.83	-21.64	-68.90	-3.91	34.14	37.01	79.66
[C4C1im][EtOEtSO4]	-42.58	47.94	-21.15	-73.29	-3.91	34.56	37.57	79.13
[C5C1im][EtOEtSO4]	-45.65	48.62	-21.08	-77.21	-3.91	34.61	37.64	79.06
[C6C1im][EtOEtSO4]	-48.76	49.43	-20.88	-81.31	-3.91	34.78	37.87	78.84
[C7C1im][EtOEtSO4]	-51.93	50.25	-20.78	-85.39	-3.91	34.86	37.97	78.74
[C8C1im][EtOEtSO4]	-55.33	51.13	-20.48	-89.63	-3.91	35.11	38.31	78.41
[C9C1im][EtOEtSO4]	-58.05	51.81	-20.47	-93.57	-3.91	35.12	38.32	78.40
[C10C1im][EtOEtSO4]	-61.39	52.80	-20.02	-97.85	-3.91	35.50	38.83	77.91
[C1C1im][MeOEtOEtSO4]	-39.27	49.77	-23.86	-67.30	-3.91	32.29	34.52	82.06
[C2C1im][MeOEtOEtSO4]	-38.46	52.02	-22.37	-70.94	-3.91	33.54	36.19	80.45
[C3C1im][MeOEtOEtSO4]	-40.81	53.03	-22.06	-74.76	-3.91	33.80	36.55	80.11
[C4C1im][MeOEtOEtSO4]	-43.62	54.04	-21.57	-79.15	-3.91	34.21	37.10	79.58
[C5C1im][MeOEtOEtSO4]	-46.78	54.65	-21.52	-83.07	-3.91	34.25	37.15	79.53
[C6C1im][MeOEtOEtSO4]	-49.96	55.41	-21.33	-87.18	-3.91	34.40	37.36	79.33
[C7C1im][MeOEtOEtSO4]	-53.19	56.19	-21.25	-91.26	-3.91	34.47	37.45	79.24
[C8C1im][MeOEtOEtSO4]	-56.63	57.02	-20.95	-95.50	-3.91	34.72	37.78	78.92
[C9C1im][MeOEtOEtSO4]	-59.41	57.66	-20.96	-99.44	-3.91	34.72	37.78	78.92
[C10C1im][MeOEtOEtSO4]	-62.75	58.65	-20.51	-103.73	-3.91	35.09	38.28	78.44
[C1C1im][SCN]	-34.66	31.54	-17.97	-48.23	-3.91	37.21	41.13	75.70
[C2C1im][SCN]	-34.13	33.78	-17.17	-51.50	-3.91	37.87	42.02	74.84
[C3C1im][SCN]	-36.38	34.83	-17.04	-55.01	-3.91	37.98	42.17	74.70
[C4C1im][SCN]	-38.89	36.10	-16.64	-59.36	-3.91	38.31	42.61	74.27
[C5C1im][SCN]	-41.76	36.96	-16.62	-63.19	-3.91	38.33	42.64	74.24
[C6C1im][SCN]	-44.54	38.03	-16.44	-67.20	-3.91	38.48	42.84	74.05
[C7C1im][SCN]	-47.48	39.08	-16.42	-71.20	-3.91	38.50	42.86	74.03
[C8C1im][SCN]	-50.73	40.18	-16.20	-75.41	-3.91	38.68	43.11	73.79
[C9C1im][SCN]	-53.18	41.09	-16.18	-79.26	-3.91	38.70	43.14	73.76
[C10C1im][SCN]	-56.44	42.23	-15.86	-83.52	-3.91	38.96	43.49	73.42

[C1C1im][N(CN)2]	-38.28	32.02	-24.04	-46.27	-3.91	32.14	34.32	82.25
[C2C1im][N(CN)2]	-36.80	34.54	-22.88	-49.18	-3.91	33.11	35.62	81.00
[C3C1im][N(CN)2]	-38.53	35.74	-22.65	-52.44	-3.91	33.30	35.88	80.75
[C4C1im][N(CN)2]	-40.89	36.99	-22.12	-56.72	-3.91	33.74	36.47	80.18
[C5C1im][N(CN)2]	-43.69	37.81	-22.07	-60.49	-3.91	33.79	36.54	80.12
[C6C1im][N(CN)2]	-46.39	38.80	-21.81	-64.41	-3.91	34.00	36.82	79.85
[C7C1im][N(CN)2]	-49.32	39.73	-21.74	-68.34	-3.91	34.06	36.90	79.77
[C8C1im][N(CN)2]	-52.54	40.72	-21.42	-72.50	-3.91	34.33	37.26	79.42
[C9C1im][N(CN)2]	-54.96	41.53	-21.37	-76.26	-3.91	34.37	37.32	79.37
[C10C1im][N(CN)2]	-58.19	42.56	-20.93	-80.49	-3.91	34.74	37.81	78.89
[C1C1im][C(CN)3]	-43.25	28.82	-18.10	-53.97	-3.91	37.10	40.98	75.84
[C2C1im][C(CN)3]	-41.06	31.67	-16.99	-56.62	-3.91	38.02	42.22	74.64
[C3C1im][C(CN)3]	-42.25	33.36	-16.82	-59.66	-3.91	38.17	42.41	74.46
[C4C1im][C(CN)3]	-44.03	34.93	-16.30	-63.80	-3.91	38.60	43.00	73.90
[C5C1im][C(CN)3]	-46.51	36.03	-16.23	-67.47	-3.91	38.65	43.07	73.83
[C6C1im][C(CN)3]	-48.95	37.19	-15.99	-71.29	-3.91	38.86	43.34	73.56
[C7C1im][C(CN)3]	-51.63	38.26	-15.87	-75.14	-3.91	38.96	43.48	73.43
[C8C1im][C(CN)3]	-54.69	39.34	-15.58	-79.22	-3.91	39.20	43.80	73.12
[C9C1im][C(CN)3]	-57.02	40.24	-15.51	-82.93	-3.91	39.25	43.88	73.05
[C10C1im][C(CN)3]	-60.13	41.28	-15.11	-87.08	-3.91	39.59	44.32	72.62
[C1C1im][B(CN)4]	-47.75	28.57	-13.76	-62.56	-3.91	40.71	45.84	71.16
[C2C1im][B(CN)4]	-45.36	31.26	-12.76	-64.84	-3.91	41.55	46.96	70.08
[C3C1im][B(CN)4]	-46.18	33.09	-12.60	-67.58	-3.91	41.68	47.14	69.91
[C4C1im][B(CN)4]	-47.61	34.74	-12.13	-71.48	-3.91	42.08	47.67	69.40
[C5C1im][B(CN)4]	-49.86	35.95	-12.04	-75.00	-3.91	42.14	47.76	69.31
[C6C1im][B(CN)4]	-52.10	37.16	-11.82	-78.66	-3.91	42.33	48.01	69.07
[C7C1im][B(CN)4]	-54.58	38.29	-11.68	-82.38	-3.91	42.45	48.17	68.92
[C8C1im][B(CN)4]	-57.50	39.40	-11.43	-86.32	-3.91	42.66	48.45	68.65

[C9C1im][B(CN)4]	-59.76	40.34	-11.36	-89.94	-3.91	42.71	48.53	68.57
[C10C1im][B(CN)4]	-62.78	41.35	-11.02	-93.97	-3.91	43.00	48.91	68.20
[C1C1im][BCIF3]	-31.90	20.87	-8.44	-44.33	-3.91	45.15	51.80	65.42
[C2C1im][BCIF3]	-29.99	24.49	-7.65	-47.81	-3.91	45.81	52.69	64.56
[C3C1im][BCIF3]	-31.21	26.80	-7.46	-51.48	-3.91	45.97	52.90	64.36
[C4C1im][BCIF3]	-32.62	29.04	-7.11	-55.80	-3.91	46.26	53.29	63.98
[C5C1im][BCIF3]	-34.75	30.70	-7.01	-59.66	-3.91	46.34	53.40	63.88
[C6C1im][BCIF3]	-37.01	32.34	-6.85	-63.71	-3.91	46.47	53.58	63.71
[C7C1im][BCIF3]	-39.41	33.88	-6.72	-67.76	-3.91	46.58	53.73	63.56
[C8C1im][BCIF3]	-42.29	35.36	-6.54	-71.97	-3.91	46.73	53.93	63.37
[C9C1im][BCIF3]	-44.54	36.61	-6.49	-75.89	-3.91	46.78	53.99	63.31
[C10C1im][BCIF3]	-47.57	37.96	-6.25	-80.14	-3.91	46.97	54.25	63.06
[C1C1im][BF4]	-22.72	25.74	-11.20	-37.26	-3.91	42.85	48.71	68.40
[C2C1im][BF4]	-21.48	28.62	-10.22	-40.74	-3.91	43.67	49.81	67.34
[C3C1im][BF4]	-23.26	30.24	-9.97	-44.41	-3.91	43.88	50.09	67.07
[C4C1im][BF4]	-25.17	31.99	-9.54	-48.75	-3.91	44.23	50.56	66.61
[C5C1im][BF4]	-27.61	33.26	-9.42	-52.61	-3.91	44.33	50.70	66.48
[C6C1im][BF4]	-30.11	34.64	-9.22	-56.67	-3.91	44.50	50.92	66.27
[C7C1im][BF4]	-32.67	35.99	-9.07	-60.72	-3.91	44.62	51.09	66.10
[C8C1im][BF4]	-35.66	37.35	-8.85	-64.94	-3.91	44.81	51.34	65.86
[C9C1im][BF4]	-37.98	38.46	-8.79	-68.86	-3.91	44.86	51.41	65.80
[C10C1im][BF4]	-41.04	39.78	-8.50	-73.12	-3.91	45.10	51.74	65.48
[C1C1im][BCl4]	-46.82	21.36	-4.81	-63.37	-3.91	48.18	55.87	61.50
[C2C1im][BCl4]	-46.12	23.92	-4.32	-66.86	-3.91	48.58	56.41	60.98
[C3C1im][BCl4]	-47.46	26.31	-4.22	-70.52	-3.91	48.67	56.53	60.87
[C4C1im][BCl4]	-48.87	28.50	-4.00	-74.79	-3.91	48.85	56.77	60.63
[C5C1im][BCl4]	-51.01	30.28	-3.94	-78.65	-3.91	48.90	56.84	60.56
[C6C1im][BCl4]	-53.33	31.89	-3.84	-82.68	-3.91	48.99	56.95	60.45

[C7C1im][BCl4]	-55.83	33.37	-3.75	-86.71	-3.91	49.06	57.05	60.36
[C8C1im][BCl4]	-58.81	34.76	-3.64	-90.90	-3.91	49.15	57.18	60.24
[C9C1im][BCl4]	-61.21	35.97	-3.60	-94.81	-3.91	49.18	57.22	60.20
[C10C1im][BCl4]	-64.40	37.13	-3.46	-99.03	-3.91	49.30	57.38	60.04
[C1C1im][PF6]	-22.83	19.05	-3.40	-38.49	-3.91	49.35	57.45	59.98
[C2C1im][PF6]	-21.02	22.85	-3.04	-41.94	-3.91	49.65	57.85	59.59
[C3C1im][PF6]	-22.00	25.58	-2.95	-45.59	-3.91	49.72	57.95	59.50
[C4C1im][PF6]	-23.22	28.07	-2.79	-49.88	-3.91	49.86	58.13	59.33
[C5C1im][PF6]	-25.22	29.97	-2.74	-53.74	-3.91	49.90	58.18	59.27
[C6C1im][PF6]	-27.40	31.75	-2.67	-57.78	-3.91	49.96	58.27	59.19
[C7C1im][PF6]	-29.77	33.38	-2.60	-61.81	-3.91	50.02	58.34	59.12
[C8C1im][PF6]	-32.65	34.93	-2.52	-66.01	-3.91	50.08	58.43	59.04
[C9C1im][PF6]	-34.92	36.25	-2.49	-69.92	-3.91	50.11	58.46	59.01
[C10C1im][PF6]	-38.01	37.58	-2.39	-74.15	-3.91	50.19	58.57	58.89
[C1C1im][AsF6]	-22.19	19.01	-2.05	-39.15	-3.91	50.48	58.96	58.52
[C2C1im][AsF6]	-20.67	22.59	-1.82	-42.59	-3.91	50.66	59.21	58.28
[C3C1im][AsF6]	-21.65	25.37	-1.77	-46.23	-3.91	50.71	59.27	58.23
[C4C1im][AsF6]	-22.87	27.87	-1.67	-50.50	-3.91	50.79	59.38	58.12
[C5C1im][AsF6]	-24.86	29.82	-1.64	-54.36	-3.91	50.82	59.42	58.08
[C6C1im][AsF6]	-27.05	31.60	-1.59	-58.38	-3.91	50.86	59.47	58.03
[C7C1im][AsF6]	-29.44	33.24	-1.55	-62.41	-3.91	50.89	59.52	57.99
[C8C1im][AsF6]	-32.34	34.77	-1.50	-66.59	-3.91	50.93	59.57	57.93
[C9C1im][AsF6]	-34.64	36.10	-1.48	-70.51	-3.91	50.95	59.59	57.91
[C10C1im][AsF6]	-37.78	37.39	-1.42	-74.73	-3.91	51.00	59.66	57.85
[C1C1im][SbF6]	-22.06	20.20	-1.94	-40.32	-3.91	50.57	59.08	58.41
[C2C1im][SbF6]	-21.12	23.14	-1.73	-43.71	-3.91	50.74	59.31	58.18
[C3C1im][SbF6]	-22.29	25.75	-1.69	-47.32	-3.91	50.78	59.36	58.14
[C4C1im][SbF6]	-23.62	28.08	-1.59	-51.57	-3.91	50.86	59.47	58.03

[C5C1im][SbF6]	-25.69	29.96	-1.56	-55.41	-3.91	50.88	59.50	58.00
[C6C1im][SbF6]	-27.96	31.65	-1.52	-59.42	-3.91	50.92	59.55	57.96
[C7C1im][SbF6]	-30.42	33.20	-1.48	-63.43	-3.91	50.95	59.59	57.91
[C8C1im][SbF6]	-33.39	34.65	-1.44	-67.60	-3.91	50.99	59.65	57.86
[C9C1im][SbF6]	-35.76	35.91	-1.42	-71.50	-3.91	51.00	59.66	57.85
[C10C1im][SbF6]	-38.96	37.12	-1.36	-75.70	-3.91	51.05	59.73	57.78
[C1C1im][BETI]	-26.53	22.07	-7.25	-41.35	-3.91	46.14	53.13	64.14
[C2C1im][BETI]	-25.77	24.80	-7.03	-44.63	-3.91	46.33	53.38	63.90
[C3C1im][BETI]	-27.19	27.12	-7.12	-48.14	-3.91	46.25	53.28	63.99
[C4C1im][BETI]	-28.71	29.25	-6.96	-52.37	-3.91	46.39	53.46	63.82
[C5C1im][BETI]	-30.99	30.92	-7.01	-56.17	-3.91	46.34	53.40	63.88
[C6C1im][BETI]	-33.36	32.46	-6.95	-60.14	-3.91	46.39	53.47	63.81
[C7C1im][BETI]	-36.00	33.85	-6.97	-64.12	-3.91	46.37	53.44	63.84
[C8C1im][BETI]	-39.09	35.18	-6.91	-68.28	-3.91	46.43	53.51	63.77
[C9C1im][BETI]	-41.51	36.33	-6.91	-72.15	-3.91	46.43	53.51	63.77
[C10C1im][BETI]	-44.76	37.45	-6.78	-76.35	-3.91	46.54	53.66	63.62
[C1C1im][Tf2N]	-34.40	29.27	-10.61	-54.32	-3.91	43.34	49.37	67.76
[C2C1im][Tf2N]	-34.08	30.92	-9.77	-57.54	-3.91	44.04	50.31	66.86
[C3C1im][Tf2N]	-36.09	32.32	-9.64	-60.99	-3.91	44.15	50.45	66.72
[C4C1im][Tf2N]	-37.99	33.77	-9.28	-65.08	-3.91	44.45	50.86	66.33
[C5C1im][Tf2N]	-40.56	34.91	-9.22	-68.78	-3.91	44.50	50.92	66.27
[C6C1im][Tf2N]	-43.16	36.02	-9.07	-72.65	-3.91	44.63	51.10	66.10
[C7C1im][Tf2N]	-45.94	37.06	-8.96	-76.54	-3.91	44.72	51.22	65.98
[C8C1im][Tf2N]	-49.07	38.08	-8.77	-80.60	-3.91	44.88	51.43	65.77
[C9C1im][Tf2N]	-51.63	38.95	-8.73	-84.40	-3.91	44.91	51.48	65.73
[C10C1im][Tf2N]	-54.86	39.89	-8.45	-88.51	-3.91	45.14	51.79	65.43
[C1C1im][Pf2N]	-34.96	32.97	-9.32	-60.18	-3.91	44.41	50.81	66.37
[C2C1im][Pf2N]	-35.26	34.03	-8.60	-63.30	-3.91	45.02	51.62	65.59



[C3C1im][Pf2N]	-37.61	35.08	-8.50	-66.66	-3.91	45.10	51.73	65.49
[C4C1im][Pf2N]	-39.73	36.23	-8.18	-70.64	-3.91	45.36	52.09	65.14
[C5C1im][Pf2N]	-42.47	37.18	-8.15	-74.27	-3.91	45.39	52.13	65.10
[C6C1im][Pf2N]	-45.19	38.10	-8.01	-78.05	-3.91	45.51	52.28	64.96
[C7C1im][Pf2N]	-48.08	38.97	-7.92	-81.87	-3.91	45.58	52.38	64.86
[C8C1im][Pf2N]	-51.31	39.84	-7.76	-85.84	-3.91	45.72	52.56	64.69
[C9C1im][Pf2N]	-53.97	40.59	-7.72	-89.58	-3.91	45.75	52.60	64.65
[C10C1im][Pf2N]	-57.29	41.38	-7.48	-93.62	-3.91	45.95	52.87	64.39
[C1C1im][Impf]	-37.49	25.45	-15.17	-48.42	-3.91	39.54	44.26	72.68
[C2C1im][Impf]	-36.74	27.63	-14.26	-51.69	-3.91	40.30	45.29	71.69
[C3C1im][Impf]	-38.48	29.30	-14.14	-55.19	-3.91	40.40	45.42	71.56
[C4C1im][Impf]	-40.32	30.96	-13.74	-59.37	-3.91	40.73	45.86	71.14
[C5C1im][Impf]	-42.85	32.19	-13.72	-63.13	-3.91	40.75	45.88	71.12
[C6C1im][Impf]	-45.41	33.40	-13.54	-67.07	-3.91	40.89	46.08	70.93
[C7C1im][Impf]	-48.21	34.50	-13.47	-71.03	-3.91	40.96	46.16	70.85
[C8C1im][Impf]	-51.34	35.60	-13.25	-75.15	-3.91	41.14	46.41	70.61
[C9C1im][Impf]	-53.84	36.52	-13.21	-78.99	-3.91	41.17	46.46	70.56
[C10C1im][Impf]	-57.07	37.52	-12.89	-83.16	-3.91	41.44	46.82	70.22
[C1C1im][Tf2C]	-37.12	29.76	-12.47	-55.40	-3.91	41.79	47.29	69.76
[C2C1im][Tf2C]	-36.98	31.38	-11.57	-58.73	-3.91	42.54	48.29	68.80
[C3C1im][Tf2C]	-39.11	32.76	-11.42	-62.28	-3.91	42.66	48.46	68.64
[C4C1im][Tf2C]	-41.08	34.21	-11.03	-66.43	-3.91	42.99	48.90	68.21
[C5C1im][Tf2C]	-43.70	35.33	-10.97	-70.17	-3.91	43.04	48.97	68.15
[C6C1im][Tf2C]	-46.35	36.43	-10.79	-74.09	-3.91	43.19	49.16	67.96
[C7C1im][Tf2C]	-49.17	37.47	-10.68	-78.03	-3.91	43.29	49.30	67.83
[C8C1im][Tf2C]	-52.33	38.50	-10.46	-82.11	-3.91	43.46	49.53	67.60
[C9C1im][Tf2C]	-54.91	39.37	-10.41	-85.95	-3.91	43.51	49.59	67.55
[C10C1im][Tf2C]	-58.16	40.31	-10.11	-90.09	-3.91	43.76	49.93	67.22

[C1C1im][Tf3C]	-37.22	31.84	-8.01	-61.37	-3.91	45.51	52.28	64.96
[C2C1im][Tf3C]	-37.67	32.88	-7.34	-64.60	-3.91	46.07	53.03	64.24
[C3C1im][Tf3C]	-40.08	33.99	-7.24	-68.07	-3.91	46.15	53.14	64.13
[C4C1im][Tf3C]	-42.19	35.20	-6.95	-72.10	-3.91	46.39	53.46	63.82
[C5C1im][Tf3C]	-44.90	36.23	-6.91	-75.76	-3.91	46.42	53.51	63.77
[C6C1im][Tf3C]	-47.63	37.21	-6.79	-79.60	-3.91	46.53	53.65	63.64
[C7C1im][Tf3C]	-50.51	38.13	-6.70	-83.45	-3.91	46.60	53.75	63.54
[C8C1im][Tf3C]	-53.73	39.05	-6.55	-87.46	-3.91	46.72	53.91	63.38
[C9C1im][Tf3C]	-56.40	39.85	-6.52	-91.23	-3.91	46.75	53.95	63.35
[C10C1im][Tf3C]	-59.73	40.66	-6.30	-95.30	-3.91	46.93	54.19	63.11

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The average absolute relative deviation, AARD, was calculated using Equation S31,

$$AARD/\% = \frac{1}{N} \sum \frac{|CA_{EXP} - CA_{PRED}|}{CA_{EXP}} \times 100\% \quad (S31)$$

where,  $N$  is the number of experimental points,  $CA_{EXP}$  is the experimental contact angle and  $CA_{PRED}$  is the respective predicted value using COSMO-RS.