

SUPPLEMENTARY INFORMATION

Prediction of the Ionic Conductivity of Imidazolium-based Ionic Liquids at Different Temperatures using Multiple Linear Regression and Support Vector Machine Algorithms

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Table S1. IL cation-anion interaction energies and dielectric energy generated using COSMO-RS

Ionic Liquids	Reference	Set	T/K	$\sigma_{exp}/S \cdot m^{-1}$	$\ln \sigma_{exp}$	Interaction Energy/ $kcal \cdot mol^{-1}$							
						$E_{MF,Cation}$	$E_{MF,Anion}$	$E_{HB,Cation}$	$E_{HB,Anion}$	$E_{vdW,Cation}$	$E_{vdW,Anion}$	$E_{Diel,Cation}$	$E_{Diel,Anion}$
[C ₄ C ₁ im][BF ₄]	[2]	Training	313.20	0.4460	-0.8074	5.1834	1.4762	-1.3746	-1.3743	-9.1328	-3.3948	-50.0718	-62.9105
[C ₄ C ₁ im][BF ₄]	[2]	Training	318.20	0.5420	-0.6125	5.2324	1.4947	-1.3519	-1.3516	-9.0807	-3.3755	-50.0718	-62.9105
[C ₄ C ₁ im][BF ₄]	[2]	Training	323.20	0.6510	-0.4292	5.2810	1.5133	-1.3285	-1.3281	-9.0277	-3.3559	-50.0718	-62.9105
[C ₄ C ₁ im][BF ₄]	[2]	Training	328.20	0.7830	-0.2446	5.3291	1.5321	-1.3044	-1.3040	-8.9740	-3.3360	-50.0718	-62.9105
[C ₆ C ₁ im][BF ₄]	[2]	Training	288.15	0.0672	-2.7001	5.1545	1.6427	-1.4300	-1.4287	-11.4416	-3.4973	-50.1150	-62.9105
[C ₆ C ₁ im][BF ₄]	[2]	Training	298.15	0.1229	-2.0964	5.2747	1.6870	-1.3894	-1.3879	-11.3270	-3.4625	-50.1150	-62.9105
[C ₆ C ₁ im][BF ₄]	[2]	Training	318.15	0.3260	-1.1209	5.5079	1.7765	-1.3001	-1.2984	-11.0822	-3.3880	-50.1150	-62.9105
[C ₆ C ₁ im][BF ₄]	[2]	Training	328.15	0.4830	-0.7277	5.6206	1.8217	-1.2517	-1.2499	-10.9533	-3.3486	-50.1150	-62.9105
[C ₆ C ₁ im][BF ₄]	[2]	Training	338.15	0.6830	-0.3813	5.7308	1.8672	-1.2011	-1.1993	-10.8208	-3.3080	-50.1150	-62.9105
[C ₆ C ₁ im][BF ₄]	[2]	Training	348.15	0.9260	-0.0769	5.8383	1.9131	-1.1487	-1.1469	-10.6854	-3.2665	-50.1150	-62.9105
[C ₆ C ₁ im][BF ₄]	[2]	Training	358.15	1.2140	0.1939	5.9430	1.9592	-1.0950	-1.0931	-10.5477	-3.2242	-50.1150	-62.9105
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	348.15	0.5360	-0.6236	8.3957	4.1484	-4.0799	-4.0634	-9.4293	-3.9096	-50.0718	-79.6259
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	338.15	0.3720	-0.9889	8.2868	4.0826	-4.2879	-4.2707	-9.5489	-3.9588	-50.0718	-79.6259
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	328.15	0.2470	-1.3984	8.1776	4.0172	-4.4893	-4.4714	-9.6658	-4.0068	-50.0718	-79.6259
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	318.15	0.1540	-1.8708	8.0686	3.9525	-4.6821	-4.6635	-9.7795	-4.0534	-50.0718	-79.6259
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	308.15	0.0830	-2.4889	7.9598	3.8888	-4.8645	-4.8452	-9.8895	-4.0984	-50.0718	-79.6259
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	298.15	0.0420	-3.1701	7.8517	3.8263	-5.0354	-5.0155	-9.9952	-4.1415	-50.0718	-79.6259
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	288.15	0.0190	-3.9633	7.7444	3.7652	-5.1942	-5.1735	-10.0962	-4.1826	-50.0718	-79.6259
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	323.15	0.2210	-1.5096	8.1231	3.9847	-4.5869	-4.5686	-9.7230	-4.0303	-50.0718	-79.6259
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	313.15	0.1310	-2.0326	8.0141	3.9206	-4.7747	-4.7557	-9.8350	-4.0761	-50.0718	-79.6259
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	303.15	0.0699	-2.6607	7.9057	3.8574	-4.9515	-4.9318	-9.9429	-4.1202	-50.0718	-79.6259
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	293.15	0.0331	-3.4082	7.7980	3.7956	-5.1163	-5.0961	-10.0463	-4.1624	-50.0718	-79.6259
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	283.15	0.0131	-4.3351	7.6911	3.7352	-5.2689	-5.2479	-10.1447	-4.2023	-50.0718	-79.6259
[C ₂ C ₁ im][C ₈ H ₁₇ SO ₄]	[2]	Training	278.10	0.0120	-4.4228	4.0829	4.8510	-2.4581	-2.4539	-7.8920	-12.7044	-50.6750	-72.5310
[C ₂ C ₁ im][C ₈ H ₁₇ SO ₄]	[2]	Training	283.10	0.0170	-4.0745	4.1256	4.9236	-2.4198	-2.4155	-7.8588	-12.6436	-50.6750	-72.5310
[C ₂ C ₁ im][C ₈ H ₁₇ SO ₄]	[2]	Training	288.10	0.0250	-3.6889	4.1681	4.9958	-2.3804	-2.3761	-7.8245	-12.5812	-50.6750	-72.5310
[C ₂ C ₁ im][C ₈ H ₁₇ SO ₄]	[2]	Training	298.10	0.0460	-3.0791	4.2526	5.1387	-2.2984	-2.2940	-7.7526	-12.4516	-50.6750	-72.5310
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	308.15	0.6570	-0.4201	5.3886	2.3907	-2.7400	-2.7289	-9.0956	-4.1631	-50.0718	-64.7784
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	313.15	0.7820	-0.2459	5.4444	2.4234	-2.6806	-2.6698	-9.0477	-4.1409	-50.0718	-64.7784

[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	328.15	1.2200	0.1989	5.6097	2.5213	-2.4972	-2.4869	-8.8985	-4.0715	-50.0718	-64.7784
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	338.15	1.5600	0.4447	5.7179	2.5865	-2.3717	-2.3618	-8.7950	-4.0232	-50.0718	-64.7784
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	343.15	1.7500	0.5596	5.7714	2.6190	-2.3084	-2.2987	-8.7422	-3.9986	-50.0718	-64.7784
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	348.15	1.9300	0.6575	5.8243	2.6515	-2.2448	-2.2354	-8.6888	-3.9737	-50.0718	-64.7784
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	353.15	1.9940	0.6901	7.4903	4.0372	-2.7385	-2.7593	-7.3406	-4.5248	-50.6750	-76.8542
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	343.15	1.5460	0.4357	7.4034	3.9887	-2.8718	-2.8931	-7.4352	-4.5831	-50.6750	-76.8542
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	333.15	1.1510	0.1406	7.3153	3.9397	-3.0010	-3.0229	-7.5279	-4.6402	-50.6750	-76.8542
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	323.15	0.8210	-0.1972	7.2263	3.8901	-3.1250	-3.1473	-7.6183	-4.6959	-50.6750	-76.8542
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	313.15	0.5530	-0.5924	7.1365	3.8401	-3.2428	-3.2655	-7.7061	-4.7498	-50.6750	-76.8542
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	308.15	0.4351	-0.8322	7.0914	3.8149	-3.2990	-3.3220	-7.7488	-4.7761	-50.6750	-76.8542
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	303.15	0.3464	-1.0602	7.0462	3.7897	-3.3535	-3.3766	-7.7906	-4.8018	-50.6750	-76.8542
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	298.15	0.2650	-1.3280	7.0009	3.7645	-3.4061	-3.4294	-7.8316	-4.8269	-50.6750	-76.8542
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	293.15	0.1972	-1.6235	6.9555	3.7392	-3.4567	-3.4802	-7.8716	-4.8514	-50.6750	-76.8542
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	278.15	0.0656	-2.7242	6.8192	3.6632	-3.5973	-3.6211	-7.9856	-4.9211	-50.6750	-76.8542
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	273.15	0.0413	-3.1859	6.7738	3.6379	-3.6404	-3.6643	-8.0214	-4.9430	-50.6750	-76.8542
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	278.15	0.2240	-1.4961	2.5275	4.6340	-0.1356	-0.1361	-6.3436	-9.5153	-50.6750	-41.7902
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	288.15	0.3620	-1.0161	2.5966	4.6914	-0.1293	-0.1297	-6.2967	-9.4329	-50.6750	-41.7902
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	308.15	0.7570	-0.2784	2.7310	4.7992	-0.1171	-0.1175	-6.1914	-9.2523	-50.6750	-41.7902
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	318.15	1.0180	0.0178	2.7964	4.8498	-0.1112	-0.1116	-6.1336	-9.1550	-50.6750	-41.7902
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	338.15	1.6580	0.5056	2.9233	4.9450	-0.0997	-0.1000	-6.0094	-8.9490	-50.6750	-41.7902
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	348.15	2.0280	0.7071	2.9848	4.9897	-0.0941	-0.0943	-5.9437	-8.8414	-50.6750	-41.7902
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	358.15	2.4290	0.8875	3.0450	5.0327	-0.0886	-0.0888	-5.8761	-8.7314	-50.6750	-41.7902
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	298.15	0.1665	-1.7928	3.6582	4.3155	-0.1127	-0.1130	-10.1368	-9.4516	-50.1150	-41.7902
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	303.15	0.2090	-1.5654	3.6945	4.3398	-0.1097	-0.1100	-10.0894	-9.4045	-50.1150	-41.7902
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	308.15	0.2580	-1.3548	3.7303	4.3636	-0.1067	-0.1070	-10.0407	-9.3563	-50.1150	-41.7902
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	313.15	0.3130	-1.1616	3.7655	4.3868	-0.1038	-0.1041	-9.9907	-9.3069	-50.1150	-41.7902
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	318.15	0.3740	-0.9835	3.8002	4.4095	-0.1009	-0.1012	-9.9396	-9.2565	-50.1150	-41.7902
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	328.15	0.5140	-0.6655	3.8679	4.4534	-0.0953	-0.0955	-9.8340	-9.1528	-50.1150	-41.7902
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	333.15	0.5930	-0.5226	3.9010	4.4746	-0.0925	-0.0927	-9.7798	-9.0996	-50.1150	-41.7902
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	338.15	0.6760	-0.3916	3.9335	4.4953	-0.0897	-0.0899	-9.7247	-9.0457	-50.1150	-41.7902
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	343.15	0.7690	-0.2627	3.9656	4.5156	-0.0870	-0.0872	-9.6687	-8.9911	-50.1150	-41.7902
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	298.10	0.3820	-0.9623	5.2897	3.3804	-2.4284	-2.4238	-7.7513	-6.3435	-50.6750	-72.0671
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	303.10	0.4850	-0.7236	5.3345	3.4132	-2.3890	-2.3844	-7.7118	-6.3098	-50.6750	-72.0671

[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	313.10	0.7200	-0.3285	5.4233	3.4781	-2.3068	-2.3022	-7.6300	-6.2402	-50.6750	-72.0671
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	318.10	0.8600	-0.1508	5.4672	3.5104	-2.2641	-2.2595	-7.5879	-6.2044	-50.6750	-72.0671
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	298.15	0.3800	-0.9676	5.2901	3.3808	-2.4280	-2.4234	-7.7509	-6.3431	-50.6750	-72.0671
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	303.15	0.4680	-0.7593	5.3349	3.4135	-2.3886	-2.3840	-7.7114	-6.3094	-50.6750	-72.0671
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	313.15	0.6750	-0.3930	5.4237	3.4784	-2.3064	-2.3018	-7.6296	-6.2399	-50.6750	-72.0671
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	318.15	0.8560	-0.1555	5.4677	3.5107	-2.2636	-2.2590	-7.5875	-6.2041	-50.6750	-72.0671
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	323.15	1.0005	0.0005	5.5113	3.5427	-2.2199	-2.2153	-7.5446	-6.1677	-50.6750	-72.0671
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	388.15	1.8560	0.6184	4.1922	4.6738	-0.3519	-0.3522	-7.6604	-8.4268	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	378.15	1.5640	0.4472	4.1262	4.5944	-0.3757	-0.3761	-7.7635	-8.5508	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	358.15	1.0500	0.0488	3.9884	4.4277	-0.4252	-0.4257	-7.9670	-8.7973	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	353.15	0.9280	-0.0747	3.9527	4.3844	-0.4378	-0.4384	-8.0170	-8.8583	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	348.15	0.8310	-0.1851	3.9164	4.3404	-0.4506	-0.4512	-8.0666	-8.9189	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	343.15	0.7240	-0.3230	3.8796	4.2956	-0.4634	-0.4640	-8.1157	-8.9791	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	338.15	0.6380	-0.4494	3.8423	4.2502	-0.4762	-0.4769	-8.1643	-9.0388	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	333.15	0.5490	-0.5997	3.8044	4.2040	-0.4890	-0.4898	-8.2123	-9.0980	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	323.15	0.4000	-0.9163	3.7270	4.1095	-0.5147	-0.5157	-8.3062	-9.2144	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	318.15	0.3364	-1.0895	3.6875	4.0611	-0.5276	-0.5286	-8.3520	-9.2716	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	308.15	0.2274	-1.4810	3.6068	3.9620	-0.5532	-0.5544	-8.4413	-9.3834	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	303.15	0.1829	-1.6988	3.5656	3.9114	-0.5659	-0.5672	-8.4845	-9.4379	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	298.15	0.1450	-1.9310	3.5239	3.8599	-0.5786	-0.5800	-8.5268	-9.4915	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	288.15	0.0853	-2.4616	3.4387	3.7547	-0.6039	-0.6055	-8.6083	-9.5954	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	283.15	0.0634	-2.7583	3.3953	3.7009	-0.6165	-0.6182	-8.6474	-9.6456	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	278.15	0.0460	-3.0791	3.3513	3.6462	-0.6291	-0.6309	-8.6854	-9.6947	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	273.15	0.0324	-3.4296	3.3067	3.5908	-0.6417	-0.6436	-8.7222	-9.7425	-50.0718	-50.3323
[C ₄ C ₁ im][PF ₆]	[2]	Training	328.15	0.5780	-0.5482	4.2267	1.7328	-0.3818	-0.3842	-8.5374	-4.0506	-50.0718	-56.5914
[C ₄ C ₁ im][PF ₆]	[2]	Training	338.15	0.8150	-0.2046	4.3108	1.7987	-0.3678	-0.3699	-8.4385	-4.0022	-50.0718	-56.5914
[C ₄ C ₁ im][PF ₆]	[2]	Training	348.15	1.1020	0.0971	4.3933	1.8652	-0.3531	-0.3550	-8.3373	-3.9527	-50.0718	-56.5914
[C ₄ C ₁ im][PF ₆]	[2]	Training	358.15	1.4400	0.3646	4.4742	1.9321	-0.3379	-0.3395	-8.2341	-3.9022	-50.0718	-56.5914
[C ₄ C ₁ im][PF ₆]	[2]	Training	368.15	1.8250	0.6016	4.5535	1.9991	-0.3222	-0.3237	-8.1294	-3.8509	-50.0718	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Training	278.15	0.0117	-4.4465	4.2679	1.6843	-0.4208	-0.4246	-11.0783	-4.2914	-50.1150	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Training	288.15	0.0270	-3.6104	4.3737	1.7474	-0.4104	-0.4138	-10.9788	-4.2523	-50.1150	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Training	293.15	0.0386	-3.2545	4.4256	1.7793	-0.4049	-0.4081	-10.9269	-4.2319	-50.1150	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Training	303.15	0.0724	-2.6255	4.5276	1.8433	-0.3934	-0.3962	-10.8191	-4.1894	-50.1150	-56.5914

[C ₆ C ₁ im][PF ₆]	[2]	Training	308.15	0.0964	-2.3392	4.5777	1.8756	-0.3873	-0.3900	-10.7632	-4.1673	-50.1150	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Training	313.15	0.1260	-2.0715	4.6271	1.9079	-0.3811	-0.3836	-10.7062	-4.1448	-50.1150	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Training	318.15	0.1612	-1.8251	4.6759	1.9403	-0.3747	-0.3771	-10.6481	-4.1218	-50.1150	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Training	333.15	0.3069	-1.1812	4.8188	2.0378	-0.3544	-0.3564	-10.4679	-4.0505	-50.1150	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Training	348.15	0.4830	-0.7277	4.9565	2.1355	-0.3328	-0.3345	-10.2803	-3.9761	-50.1150	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Training	328.15	0.2640	-1.3318	4.7718	2.0052	-0.3614	-0.3635	-10.5289	-4.0746	-50.1150	-56.5914
[C ₃ C ₁ im][SCN]	[2]	Training	323.15	1.3300	0.2852	5.9240	1.7147	-1.8826	-1.8753	-9.4318	-4.5864	-50.1735	-64.8886
[C ₃ C ₁ im][SCN]	[2]	Training	318.15	1.1000	0.0953	5.8763	1.6946	-1.9274	-1.9198	-9.4826	-4.6077	-50.1735	-64.8886
[C ₃ C ₁ im][SCN]	[2]	Training	313.15	0.9050	-0.0998	5.8281	1.6746	-1.9718	-1.9640	-9.5323	-4.6284	-50.1735	-64.8886
[C ₃ C ₁ im][SCN]	[2]	Training	308.15	0.7330	-0.3106	5.7794	1.6545	-2.0158	-2.0078	-9.5808	-4.6485	-50.1735	-64.8886
[C ₃ C ₁ im][SCN]	[2]	Training	303.15	0.5830	-0.5396	5.7302	1.6344	-2.0594	-2.0512	-9.6282	-4.6679	-50.1735	-64.8886
[C ₃ C ₁ im][SCN]	[2]	Training	298.15	0.4590	-0.7787	5.6806	1.6143	-2.1025	-2.0942	-9.6743	-4.6866	-50.1735	-64.8886
[C ₃ C ₁ im][SCN]	[2]	Training	293.15	0.3610	-1.0189	5.6305	1.5943	-2.1452	-2.1367	-9.7190	-4.7045	-50.1735	-64.8886
[C ₂ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	293.15	0.7520	-0.2850	3.0226	3.1181	-0.7791	-0.7795	-6.8226	-7.7581	-50.6750	-52.0438
[C ₂ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	313.15	1.3500	0.3001	3.1802	3.3092	-0.7204	-0.7206	-6.6915	-7.5818	-50.6750	-52.0438
[C ₂ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	333.15	2.1000	0.7419	3.3325	3.4932	-0.6592	-0.6592	-6.5487	-7.3937	-50.6750	-52.0438
[C ₂ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	353.15	3.0500	1.1151	3.4791	3.6700	-0.5964	-0.5962	-6.3971	-7.1972	-50.6750	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	298.15	0.4030	-0.9088	3.6487	3.1844	-0.7358	-0.7364	-8.7570	-7.7428	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	323.15	0.9100	-0.0943	3.8664	3.4136	-0.6598	-0.6601	-8.5329	-7.5163	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	348.15	1.6200	0.4824	4.0708	3.6303	-0.5817	-0.5818	-8.2887	-7.2742	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	301.15	0.4525	-0.7930	3.6756	3.2126	-0.7268	-0.7274	-8.7314	-7.7167	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	303.15	0.4876	-0.7183	3.6933	3.2312	-0.7208	-0.7214	-8.7141	-7.6991	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	305.15	0.5244	-0.6455	3.7110	3.2498	-0.7148	-0.7154	-8.6967	-7.6814	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	308.15	0.5812	-0.5427	3.7374	3.2776	-0.7058	-0.7062	-8.6702	-7.6545	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	313.15	0.6839	-0.3799	3.7810	3.3234	-0.6906	-0.6910	-8.6253	-7.6092	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	318.15	0.7955	-0.2288	3.8240	3.3688	-0.6753	-0.6756	-8.5795	-7.5631	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	328.15	1.0750	0.0723	3.9084	3.4580	-0.6443	-0.6446	-8.4854	-7.4689	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	333.15	1.2420	0.2167	3.9498	3.5018	-0.6287	-0.6289	-8.4372	-7.4210	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	353.15	1.9770	0.6816	4.1100	3.6721	-0.5660	-0.5661	-8.2380	-7.2244	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	273.15	0.1180	-2.1371	3.4177	2.9425	-0.8087	-0.8098	-8.9542	-7.9471	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	288.15	0.2590	-1.3509	3.5579	3.0891	-0.7653	-0.7661	-8.8394	-7.8275	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	293.15	0.3230	-1.1301	3.6036	3.1370	-0.7506	-0.7513	-8.7988	-7.7856	-50.0718	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	278.15	0.0776	-2.5562	3.8926	3.0208	-0.7763	-0.7762	-10.9313	-7.9313	-50.1150	-52.0438

[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	288.15	0.1359	-1.9958	3.9961	3.1173	-0.7464	-0.7461	-10.8343	-7.8506	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	298.15	0.2178	-1.5242	4.0968	3.2114	-0.7161	-0.7157	-10.7316	-7.7659	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	308.15	0.3275	-1.1163	4.1948	3.3033	-0.6855	-0.6850	-10.6236	-7.6777	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	318.15	0.4660	-0.7636	4.2899	3.3930	-0.6545	-0.6540	-10.5109	-7.5864	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	328.15	0.6340	-0.4557	4.3823	3.4804	-0.6233	-0.6227	-10.3941	-7.4923	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	338.15	0.8300	-0.1863	4.4719	3.5656	-0.5919	-0.5913	-10.2736	-7.3959	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	348.15	1.0540	0.0526	4.5589	3.6486	-0.5606	-0.5599	-10.1500	-7.2976	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	368.15	1.5790	0.4568	4.7250	3.8083	-0.4986	-0.4980	-9.8960	-7.0970	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	378.15	1.8750	0.6286	4.8042	3.8850	-0.4685	-0.4678	-9.7665	-6.9955	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	388.15	2.1920	0.7848	4.8809	3.9597	-0.4391	-0.4385	-9.6361	-6.8936	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	398.15	2.5260	0.9266	4.9553	4.0325	-0.4107	-0.4101	-9.5051	-6.7917	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	293.15	0.1700	-1.7720	4.0468	3.1646	-0.7313	-0.7310	-10.7837	-7.8087	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	303.15	0.2700	-1.3093	4.1461	3.2576	-0.7008	-0.7004	-10.6782	-7.7223	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	313.15	0.3900	-0.9416	4.2427	3.3484	-0.6700	-0.6695	-10.5678	-7.6324	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	333.15	0.7200	-0.3285	4.4275	3.5233	-0.6076	-0.6070	-10.3342	-7.4443	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	353.15	1.2000	0.1823	4.6014	3.6893	-0.5450	-0.5443	-10.0873	-7.2479	-50.1150	-52.0438
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	283.15	0.1020	-2.2828	3.9447	3.0693	-0.7614	-0.7612	-10.8836	-7.8915	-50.1150	-52.0438
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	278.15	0.7020	-0.3538	3.4065	2.5715	-1.2494	-1.2461	-7.9250	-8.4625	-50.6750	-49.0681
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	283.15	0.8840	-0.1233	3.4481	2.6096	-1.2257	-1.2224	-7.8875	-8.4275	-50.6750	-49.0681
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	288.15	1.0880	0.0843	3.4894	2.6477	-1.2019	-1.1987	-7.8491	-8.3912	-50.6750	-49.0681
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	298.15	1.5560	0.4421	3.5706	2.7234	-1.1540	-1.1510	-7.7698	-8.3153	-50.6750	-49.0681
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	303.15	1.8080	0.5922	3.6107	2.7612	-1.1299	-1.1270	-7.7289	-8.2756	-50.6750	-49.0681
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	313.15	2.3790	0.8667	3.6897	2.8362	-1.0814	-1.0786	-7.6448	-8.1933	-50.6750	-49.0681
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	323.15	3.0120	1.1026	3.7671	2.9108	-1.0326	-1.0299	-7.5579	-8.1071	-50.6750	-49.0681
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	333.15	3.6940	1.3067	3.8430	2.9848	-0.9834	-0.9809	-7.4687	-8.0177	-50.6750	-49.0681
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	343.15	4.4120	1.4843	3.9172	3.0581	-0.9342	-0.9318	-7.3775	-7.9253	-50.6750	-49.0681
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	353.15	5.1000	1.6292	3.9899	3.1308	-0.8851	-0.8829	-7.2846	-7.8305	-50.6750	-49.0681
[C ₈ C ₁ im][BF ₄]	[2]	Training	298.15	0.0587	-2.8353	5.5598	1.9144	-1.3489	-1.3492	-13.3892	-3.4725	-50.2776	-62.9105
[C ₈ C ₁ im][BF ₄]	[2]	Training	348.15	0.4860	-0.7215	6.1801	2.1679	-1.1039	-1.1035	-12.6341	-3.2767	-50.2776	-62.9105
[C ₈ C ₁ im][BF ₄]	[2]	Training	308.15	0.1012	-2.2907	5.6901	1.9652	-1.3041	-1.3043	-13.2482	-3.4361	-50.2776	-62.9105
[C ₈ C ₁ im][BF ₄]	[2]	Training	318.15	0.1647	-1.8036	5.8173	2.0159	-1.2570	-1.2570	-13.1014	-3.3981	-50.2776	-62.9105
[C ₈ C ₁ im][BF ₄]	[2]	Training	328.15	0.2520	-1.3783	5.9414	2.0666	-1.2077	-1.2076	-12.9497	-3.3587	-50.2776	-62.9105
[C ₈ C ₁ im][BF ₄]	[2]	Training	338.15	0.3680	-0.9997	6.0624	2.1173	-1.1566	-1.1562	-12.7937	-3.3182	-50.2776	-62.9105

[C ₈ C ₁ im][BF ₄]	[2]	Training	358.15	0.6880	-0.3740	6.2946	2.2185	-1.0502	-1.0496	-12.4718	-3.2344	-50.2776	-62.9105
[C ₂ C ₁ im][C(CN) ₃]	[2]	Training	298.00	0.7600	-0.2744	4.1115	2.2590	-1.7579	-1.7536	-7.7816	-6.4099	-50.6750	-53.5982
[C ₂ C ₁ im][C(CN) ₃]	[2]	Training	313.00	1.2500	0.2231	4.2426	2.3603	-1.6568	-1.6526	-7.6618	-6.3273	-50.6750	-53.5982
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	268.15	0.0539	-2.9206	4.2538	2.0489	-1.8747	-1.8731	-9.3551	-5.1213	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	288.15	0.1808	-1.7104	4.4701	2.1896	-1.7584	-1.7565	-9.1971	-5.0306	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	298.15	0.2900	-1.2379	4.5758	2.2598	-1.6966	-1.6945	-9.1104	-4.9808	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	308.15	0.4360	-0.8301	4.6798	2.3298	-1.6323	-1.6302	-9.0192	-4.9284	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	318.15	0.6210	-0.4764	4.7820	2.3994	-1.5659	-1.5637	-8.9238	-4.8736	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	348.15	1.4260	0.3549	5.0760	2.6051	-1.3567	-1.3545	-8.6183	-4.6981	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	358.15	1.7750	0.5738	5.1696	2.6723	-1.2853	-1.2831	-8.5115	-4.6368	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	368.15	2.1600	0.7701	5.2610	2.7388	-1.2141	-1.2120	-8.4030	-4.5745	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	293.15	0.2300	-1.4697	4.5232	2.2248	-1.7278	-1.7258	-9.1543	-5.0061	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	313.15	0.5200	-0.6539	4.7311	2.3647	-1.5994	-1.5972	-8.9720	-4.9013	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	333.15	0.9400	-0.0619	4.9314	2.5029	-1.4627	-1.4605	-8.7743	-4.7877	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	353.15	1.6000	0.4700	5.1231	2.6388	-1.3210	-1.3188	-8.5651	-4.6676	-50.0718	-60.9237
[C ₈ C ₁ im][PF ₆]	[2]	Training	283.15	0.0081	-4.8196	4.7573	1.9284	-0.3996	-0.4036	-13.1300	-4.2909	-50.2776	-56.5914
[C ₈ C ₁ im][PF ₆]	[2]	Training	288.15	0.0121	-4.4129	4.8148	1.9606	-0.3941	-0.3979	-13.0696	-4.2709	-50.2776	-56.5914
[C ₈ C ₁ im][PF ₆]	[2]	Training	298.15	0.0252	-3.6809	4.9272	2.0251	-0.3825	-0.3860	-12.9438	-4.2293	-50.2776	-56.5914
[C ₈ C ₁ im][PF ₆]	[2]	Training	303.15	0.0353	-3.3439	4.9822	2.0574	-0.3765	-0.3798	-12.8785	-4.2077	-50.2776	-56.5914
[C ₈ C ₁ im][PF ₆]	[2]	Training	308.15	0.0479	-3.0386	5.0365	2.0896	-0.3704	-0.3734	-12.8117	-4.1856	-50.2776	-56.5914
[C ₈ C ₁ im][PF ₆]	[2]	Training	313.15	0.0653	-2.7288	5.0899	2.1219	-0.3641	-0.3669	-12.7435	-4.1629	-50.2776	-56.5914
[C ₈ C ₁ im][PF ₆]	[2]	Training	318.15	0.0858	-2.4557	5.1426	2.1542	-0.3576	-0.3603	-12.6740	-4.1399	-50.2776	-56.5914
[C ₈ C ₁ im][PF ₆]	[2]	Training	323.15	0.1108	-2.2000	5.1946	2.1864	-0.3510	-0.3535	-12.6032	-4.1164	-50.2776	-56.5914
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	293.15	0.1000	-2.3026	4.4377	3.1950	-0.7158	-0.7169	-12.7935	-7.8273	-50.2776	-52.0438
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	298.15	0.1300	-2.0402	4.4918	3.2412	-0.7003	-0.7012	-12.7311	-7.7845	-50.2776	-52.0438
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	303.15	0.1600	-1.8326	4.5450	3.2868	-0.6847	-0.6855	-12.6672	-7.7409	-50.2776	-52.0438
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	313.15	0.2400	-1.4271	4.6490	3.3761	-0.6533	-0.6540	-12.5351	-7.6512	-50.2776	-52.0438
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	333.15	0.4700	-0.7550	4.8470	3.5476	-0.5902	-0.5906	-12.2557	-7.4634	-50.2776	-52.0438
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	353.15	0.8000	-0.2231	5.0322	3.7097	-0.5274	-0.5276	-11.9605	-7.2671	-50.2776	-52.0438
[C ₄ C ₁ im][BF ₄]	[2]	Test	308.20	0.3640	-1.0106	5.1338	1.4579	-1.3965	-1.3964	-9.1840	-3.4137	-50.0718	-62.9105
[C ₆ C ₁ im][BF ₄]	[2]	Test	308.15	0.2070	-1.5750	5.3925	1.7316	-1.3461	-1.3445	-11.2070	-3.4261	-50.1150	-62.9105
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Test	358.15	0.7360	-0.3065	8.5041	4.2146	-3.8675	-3.8518	-9.3077	-3.8594	-50.0718	-79.6259
[C ₂ C ₁ im][C ₈ H ₁₇ SO ₄]	[2]	Test	293.10	0.0340	-3.3814	4.2105	5.0675	-2.3399	-2.3355	-7.7890	-12.5172	-50.6750	-72.5310

[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Test	298.15	0.4550	-0.7875	5.2761	2.3257	-2.8555	-2.8441	-9.1882	-4.2060	-50.0718	-64.7784
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Test	303.15	0.5470	-0.6033	5.3325	2.3582	-2.7983	-2.7871	-9.1424	-4.1848	-50.0718	-64.7784
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Test	318.15	0.9200	-0.0834	5.4999	2.4560	-2.6203	-2.6096	-8.9989	-4.1182	-50.0718	-64.7784
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Test	323.15	1.0500	0.0488	5.5550	2.4887	-2.5592	-2.5486	-8.9491	-4.0950	-50.0718	-64.7784
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Test	333.15	1.3800	0.3221	5.6641	2.5539	-2.4347	-2.4246	-8.8471	-4.0475	-50.0718	-64.7784
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Test	288.15	0.1420	-1.9519	6.9101	3.7139	-3.5055	-3.5291	-7.9107	-4.8753	-50.6750	-76.8542
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Test	283.15	0.0988	-2.3147	6.8647	3.6885	-3.5523	-3.5761	-7.9487	-4.8986	-50.6750	-76.8542
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Test	298.15	0.5390	-0.6180	2.6644	4.7464	-0.1231	-0.1236	-6.2459	-9.3451	-50.6750	-41.7902
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Test	328.15	1.3180	0.2761	2.8605	4.8983	-0.1054	-0.1057	-6.0728	-9.0537	-50.6750	-41.7902
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Test	293.15	0.1303	-2.0379	3.6212	4.2907	-0.1158	-0.1161	-10.1828	-9.4975	-50.1150	-41.7902
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Test	323.15	0.4400	-0.8210	3.8343	4.4317	-0.0981	-0.0983	-9.8873	-9.2051	-50.1150	-41.7902
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Test	308.10	0.6100	-0.4943	5.3790	3.4457	-2.3485	-2.3439	-7.6713	-6.2753	-50.6750	-72.0671
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Test	308.15	0.5660	-0.5692	5.3795	3.4460	-2.3481	-2.3435	-7.6709	-6.2750	-50.6750	-72.0671
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Test	368.15	1.2930	0.2570	4.0583	4.5124	-0.4002	-0.4006	-7.8658	-8.6744	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Test	328.15	0.4747	-0.7451	3.7660	4.1571	-0.5019	-0.5027	-8.2596	-9.1565	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Test	313.15	0.2780	-1.2801	3.6474	4.0119	-0.5404	-0.5415	-8.3971	-9.3279	-50.0718	-50.3323
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Test	293.15	0.1122	-2.1875	3.4816	3.8077	-0.5913	-0.5928	-8.5681	-9.5440	-50.0718	-50.3323
[C ₆ C ₁ im][PF ₆]	[2]	Test	283.15	0.0184	-3.9981	4.3211	1.7157	-0.4157	-0.4193	-11.0293	-4.2722	-50.1150	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Test	298.15	0.0519	-2.9584	4.4769	1.8112	-0.3992	-0.4022	-10.8737	-4.2109	-50.1150	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Test	343.15	0.4510	-0.7963	4.9112	2.1029	-0.3402	-0.3419	-10.3435	-4.0012	-50.1150	-56.5914
[C ₆ C ₁ im][PF ₆]	[2]	Test	323.15	0.2120	-1.5512	4.7242	1.9727	-0.3681	-0.3703	-10.5890	-4.0984	-50.1150	-56.5914
[C ₃ C ₁ im][SCN]	[2]	Test	288.15	0.2550	-1.3665	5.5800	1.5742	-2.1873	-2.1786	-9.7624	-4.7217	-50.1735	-64.8886
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Test	283.15	0.2070	-1.5750	3.5117	3.0408	-0.7799	-0.7808	-8.8789	-7.8684	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Test	311.15	0.6429	-0.4418	3.7636	3.3052	-0.6967	-0.6971	-8.6434	-7.6274	-50.0718	-52.0438
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Test	278.15	0.1580	-1.8452	3.4649	2.9919	-0.7943	-0.7954	-8.9172	-7.9083	-50.0718	-52.0438
[C ₂ C ₁ im][B(CN) ₄]	[2]	Test	273.15	0.5450	-0.6070	3.3646	2.5332	-1.2730	-1.2697	-7.9615	-8.4962	-50.6750	-49.0681
[C ₂ C ₁ im][B(CN) ₄]	[2]	Test	293.15	1.3110	0.2708	3.5302	2.6856	-1.1780	-1.1749	-7.8099	-8.3538	-50.6750	-49.0681
[C ₈ C ₁ im][BF ₄]	[2]	Test	323.15	0.2030	-1.5945	5.8798	2.0413	-1.2327	-1.2325	-13.0261	-3.3786	-50.2776	-62.9105
[C ₈ C ₁ im][BF ₄]	[2]	Test	288.15	0.0304	-3.4933	5.4266	1.8635	-1.3911	-1.3917	-13.5239	-3.5072	-50.2776	-62.9105
[C ₂ C ₁ im][C(CN) ₃]	[2]	Test	303.00	0.9300	-0.0726	4.1556	2.2929	-1.7247	-1.7204	-7.7425	-6.3831	-50.6750	-53.5982
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Test	278.15	0.1038	-2.2653	4.3627	2.1193	-1.8178	-1.8160	-9.2788	-5.0775	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Test	328.15	0.8480	-0.1649	4.8821	2.4685	-1.4975	-1.4953	-8.8249	-4.8168	-50.0718	-60.9237
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Test	338.15	1.1170	0.1106	4.9801	2.5371	-1.4276	-1.4254	-8.7229	-4.7582	-50.0718	-60.9237

[C ₈ C ₁ im][PF ₆]	[2]	Test	293.15	0.0177	-4.0342	4.8714	1.9928	-0.3884	-0.3920	-13.0075	-4.2504	-50.2776	-56.5914
[C ₈ C ₁ im][PF ₆]	[2]	Test	348.15	0.2900	-1.2379	5.4432	2.3464	-0.3158	-0.3177	-12.2339	-3.9936	-50.2776	-56.5914
[C ₄ C ₁ im][CH ₃ SO ₄]	[97]	Test	333.15	0.6230	-0.4732	6.1318	3.1974	-2.0100	-2.0076	-9.4037	-5.0726	-50.0718	-71.0882
[C ₄ C ₁ im][CH ₃ SO ₄]	[97]	Test	343.15	0.8840	-0.1233	6.2338	3.2533	-1.9196	-1.9171	-9.2893	-5.0098	-50.0718	-71.0882
[C ₂ C ₁ im][CH ₃ CO ₂]	[98]	Test	338.15	1.4770	0.3900	8.4374	3.9827	-4.3854	-4.3657	-7.6077	-3.9598	-50.6750	-79.6259
[C ₂ C ₁ im][CH ₃ CO ₂]	[98]	Test	348.15	1.9560	0.6709	8.5318	4.0385	-4.1768	-4.1580	-7.5117	-3.9108	-50.6750	-79.6259
[C ₂ C ₁ im][CH ₃ CO ₂]	[98]	Test	358.15	2.5030	0.9175	8.6256	4.0946	-3.9637	-3.9457	-7.4140	-3.8608	-50.6750	-79.6259
[C ₃ C ₁ im][N(CF ₃ SO ₂) ₂]	[99]	Test	283.00	0.3210	-1.1363	3.2567	3.0250	-0.7892	-0.7902	-7.8878	-7.8557	-50.1735	-52.0438
[C ₃ C ₁ im][N(CF ₃ SO ₂) ₂]	[99]	Test	292.00	0.4770	-0.7402	3.3345	3.1123	-0.7633	-0.7642	-7.8247	-7.7815	-50.1735	-52.0438
[C ₃ C ₁ im][N(CF ₃ SO ₂) ₂]	[99]	Test	303.00	0.7100	-0.3425	3.4276	3.2170	-0.7311	-0.7318	-7.7432	-7.6866	-50.1735	-52.0438
[C ₃ C ₁ im][N(CF ₃ SO ₂) ₂]	[99]	Test	313.00	0.9710	-0.0294	3.5103	3.3102	-0.7013	-0.7018	-7.6652	-7.5968	-50.1735	-52.0438
[C ₃ C ₁ im][N(CF ₃ SO ₂) ₂]	[99]	Test	323.00	1.2520	0.2247	3.5913	3.4015	-0.6708	-0.6712	-7.5839	-7.5040	-50.1735	-52.0438

Table S2. Predicted ionic conductivity values using MLR and SVM regression algorithm

Ionic Liquids	Reference	Set	T/K	$\sigma_{exp}/S \cdot m^{-1}$	$\ln \sigma_{exp}$	MLR Algorithm			SVM Regression Algorithm		
						$\ln \sigma_{pred}$	$\sigma_{pred}/S \cdot m^{-1}$	$ \% \Delta E $	$\ln \sigma_{pred}$	$\sigma_{pred}/S \cdot m^{-1}$	$ \% \Delta E $
[C ₄ C ₁ im][BF ₄]	[2]	Training	313.20	0.4460	-0.8074	-0.5514	0.5762	29.18%	-0.7116	0.4909	10.06%
[C ₄ C ₁ im][BF ₄]	[2]	Training	318.20	0.5420	-0.6125	-0.3255	0.7221	33.23%	-0.5086	0.6014	10.95%
[C ₄ C ₁ im][BF ₄]	[2]	Training	323.20	0.6510	-0.4292	-0.1054	0.8999	38.24%	-0.3221	0.7247	11.31%
[C ₄ C ₁ im][BF ₄]	[2]	Training	328.20	0.7830	-0.2446	0.1091	1.1153	42.44%	-0.1506	0.8602	9.86%
[C ₆ C ₁ im][BF ₄]	[2]	Training	288.15	0.0672	-2.7001	-2.8629	0.0571	15.03%	-2.8307	0.0590	12.24%
[C ₆ C ₁ im][BF ₄]	[2]	Training	298.15	0.1229	-2.0964	-2.3347	0.0968	21.21%	-2.1500	0.1165	5.22%
[C ₆ C ₁ im][BF ₄]	[2]	Training	318.15	0.3260	-1.1209	-1.3565	0.2576	20.99%	-1.0932	0.3351	2.80%
[C ₆ C ₁ im][BF ₄]	[2]	Training	328.15	0.4830	-0.7277	-0.9025	0.4056	16.03%	-0.6876	0.5028	4.09%
[C ₆ C ₁ im][BF ₄]	[2]	Training	338.15	0.6830	-0.3813	-0.4695	0.6253	8.45%	-0.3461	0.7075	3.58%
[C ₆ C ₁ im][BF ₄]	[2]	Training	348.15	0.9260	-0.0769	-0.0563	0.9452	2.08%	-0.0572	0.9444	1.98%
[C ₆ C ₁ im][BF ₄]	[2]	Training	358.15	1.2140	0.1939	0.3384	1.4027	15.54%	0.1883	1.2073	0.56%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	348.15	0.5360	-0.6236	-0.6228	0.5364	0.08%	-0.5667	0.5674	5.85%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	338.15	0.3720	-0.9889	-1.0076	0.3651	1.85%	-0.9423	0.3897	4.77%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	328.15	0.2470	-1.3984	-1.4102	0.2441	1.18%	-1.3717	0.2537	2.71%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	318.15	0.1540	-1.8708	-1.8322	0.1601	3.94%	-1.8650	0.1549	0.59%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	308.15	0.0830	-2.4889	-2.2751	0.1028	23.84%	-2.4342	0.0877	5.62%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	298.15	0.0420	-3.1701	-2.7409	0.0645	53.60%	-3.0929	0.0454	8.02%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	288.15	0.0190	-3.9633	-3.2319	0.0395	107.79%	-3.8554	0.0212	11.40%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	323.15	0.2210	-1.5096	-1.6187	0.1982	10.34%	-1.6096	0.2000	9.52%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	313.15	0.1310	-2.0326	-2.0509	0.1286	1.82%	-2.1393	0.1177	10.12%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	303.15	0.0699	-2.6607	-2.5050	0.0817	16.85%	-2.7515	0.0638	8.68%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	293.15	0.0331	-3.4082	-2.9831	0.0506	52.98%	-3.4603	0.0314	5.07%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Training	283.15	0.0131	-4.3351	-3.4877	0.0306	133.36%	-4.2799	0.0138	5.68%
[C ₂ C ₁ im][C ₈ H ₁₇ SO ₄]	[2]	Training	278.10	0.0120	-4.4228	-3.1588	0.0425	253.99%	-4.3259	0.0132	10.18%
[C ₂ C ₁ im][C ₈ H ₁₇ SO ₄]	[2]	Training	283.10	0.0170	-4.0745	-2.9662	0.0515	202.93%	-4.0211	0.0179	5.49%
[C ₂ C ₁ im][C ₈ H ₁₇ SO ₄]	[2]	Training	288.10	0.0250	-3.6889	-2.7811	0.0620	147.89%	-3.7300	0.0240	4.03%
[C ₂ C ₁ im][C ₈ H ₁₇ SO ₄]	[2]	Training	298.10	0.0460	-3.0791	-2.4313	0.0879	91.13%	-3.1863	0.0413	10.16%
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	308.15	0.6570	-0.4201	-1.3413	0.2615	60.20%	-0.5278	0.5899	10.21%
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	313.15	0.7820	-0.2459	-1.1201	0.3263	58.28%	-0.3331	0.7167	8.35%

[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	328.15	1.2200	0.1989	-0.4895	0.6129	49.76%	0.1555	1.1682	4.24%
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	338.15	1.5600	0.4447	-0.0947	0.9096	41.69%	0.4167	1.5170	2.76%
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	343.15	1.7500	0.5596	0.0956	1.1003	37.12%	0.5319	1.7022	2.73%
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Training	348.15	1.9300	0.6575	0.2814	1.3250	31.35%	0.6383	1.8932	1.91%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	353.15	1.9940	0.6901	0.8095	2.2469	12.68%	0.6737	1.9614	1.64%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	343.15	1.5460	0.4357	0.4531	1.5732	1.76%	0.4053	1.4998	2.99%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	333.15	1.1510	0.1406	0.0793	1.0826	5.94%	0.0955	1.1002	4.42%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	323.15	0.8210	-0.1972	-0.3131	0.7312	10.94%	-0.2633	0.7685	6.39%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	313.15	0.5530	-0.5924	-0.7257	0.4840	12.48%	-0.6795	0.5068	8.35%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	308.15	0.4351	-0.8322	-0.9402	0.3906	10.24%	-0.9124	0.4016	7.71%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	303.15	0.3464	-1.0602	-1.1604	0.3134	9.54%	-1.1636	0.3124	9.83%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	298.15	0.2650	-1.3280	-1.3867	0.2499	5.70%	-1.4347	0.2382	10.11%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	293.15	0.1972	-1.6235	-1.6193	0.1980	0.42%	-1.7271	0.1778	9.83%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	278.15	0.0656	-2.7242	-2.3586	0.0946	44.13%	-2.7481	0.0641	2.36%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Training	273.15	0.0413	-3.1859	-2.6201	0.0728	76.10%	-3.1413	0.0432	4.56%
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	278.15	0.2240	-1.4961	-1.5405	0.2143	4.34%	-1.6031	0.2013	10.15%
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	288.15	0.3620	-1.0161	-1.0932	0.3351	7.42%	-1.0925	0.3354	7.36%
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	308.15	0.7570	-0.2784	-0.2795	0.7562	0.11%	-0.2691	0.7641	0.94%
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	318.15	1.0180	0.0178	0.0920	1.0964	7.70%	0.0609	1.0628	4.41%
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	338.15	1.6580	0.5056	0.7745	2.1696	30.86%	0.5940	1.8112	9.24%
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	348.15	2.0280	0.7071	1.0890	2.9714	46.52%	0.8087	2.2450	10.70%
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	358.15	2.4290	0.8875	1.3876	4.0053	64.89%	0.9951	2.7049	11.36%
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	298.15	0.1665	-1.7928	-1.7871	0.1675	0.57%	-1.8997	0.1496	10.15%
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	303.15	0.2090	-1.5654	-1.5716	0.2077	0.61%	-1.6472	0.1926	7.85%
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	308.15	0.2580	-1.3548	-1.3621	0.2561	0.72%	-1.4125	0.2435	5.61%
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	313.15	0.3130	-1.1616	-1.1583	0.3140	0.33%	-1.1941	0.3030	3.21%
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	318.15	0.3740	-0.9835	-0.9599	0.3829	2.39%	-0.9907	0.3713	0.72%
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	328.15	0.5140	-0.6655	-0.5785	0.5607	9.09%	-0.6236	0.5360	4.29%
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	333.15	0.5930	-0.5226	-0.3951	0.6736	13.60%	-0.4575	0.6329	6.72%
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	338.15	0.6760	-0.3916	-0.2162	0.8056	19.17%	-0.3017	0.7395	9.40%
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Training	343.15	0.7690	-0.2627	-0.0417	0.9592	24.73%	-0.1553	0.8561	11.33%
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	298.10	0.3820	-0.9623	-1.6325	0.1954	48.84%	-0.8627	0.4220	10.48%
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	303.10	0.4850	-0.7236	-1.4171	0.2424	50.02%	-0.6844	0.5044	4.00%

[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	313.10	0.7200	-0.3285	-1.0046	0.3662	49.14%	-0.3719	0.6894	4.25%
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	318.10	0.8600	-0.1508	-0.8068	0.4463	48.11%	-0.2348	0.7907	8.05%
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	298.15	0.3800	-0.9676	-1.6303	0.1959	48.46%	-0.8608	0.4228	11.27%
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	303.15	0.4680	-0.7593	-1.4150	0.2429	48.09%	-0.6827	0.5053	7.96%
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	313.15	0.6750	-0.3930	-1.0026	0.3669	45.64%	-0.3705	0.6904	2.28%
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	318.15	0.8560	-0.1555	-0.8049	0.4472	47.76%	-0.2335	0.7918	7.50%
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Training	323.15	1.0005	0.0005	-0.6125	0.5420	45.83%	-0.1073	0.8983	10.22%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	388.15	1.8560	0.6184	1.2168	3.3762	81.91%	0.5559	1.7436	6.06%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	378.15	1.5640	0.4472	0.9756	2.6528	69.61%	0.3699	1.4476	7.44%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	358.15	1.0500	0.0488	0.4559	1.5776	50.25%	-0.0521	0.9492	9.60%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	353.15	0.9280	-0.0747	0.3174	1.3736	48.02%	-0.1697	0.8439	9.06%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	348.15	0.8310	-0.1851	0.1753	1.1916	43.39%	-0.2927	0.7462	10.20%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	343.15	0.7240	-0.3230	0.0293	1.0297	42.22%	-0.4217	0.6559	9.41%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	338.15	0.6380	-0.4494	-0.1208	0.8862	38.90%	-0.5573	0.5727	10.23%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	333.15	0.5490	-0.5997	-0.2751	0.7595	38.35%	-0.7000	0.4966	9.55%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	323.15	0.4000	-0.9163	-0.5971	0.5504	37.61%	-1.0098	0.3643	8.92%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	318.15	0.3364	-1.0895	-0.7652	0.4653	38.30%	-1.1785	0.3077	8.52%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	308.15	0.2274	-1.4810	-1.1169	0.3273	43.93%	-1.5485	0.2126	6.53%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	303.15	0.1829	-1.6988	-1.3011	0.2722	48.85%	-1.7522	0.1734	5.20%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	298.15	0.1450	-1.9310	-1.4911	0.2251	55.26%	-1.9700	0.1395	3.82%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	288.15	0.0853	-2.4616	-1.8900	0.1511	77.10%	-2.4537	0.0860	0.79%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	283.15	0.0634	-2.7583	-2.0996	0.1225	93.22%	-2.7225	0.0657	3.64%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	278.15	0.0460	-3.0791	-2.3166	0.0986	114.38%	-3.0115	0.0492	6.99%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Training	273.15	0.0324	-3.4296	-2.5412	0.0788	143.13%	-3.3221	0.0361	11.35%
[C ₄ C ₁ im][PF ₆]	[2]	Training	328.15	0.5780	-0.5482	-0.0358	0.9649	66.93%	-0.6541	0.5199	10.05%
[C ₄ C ₁ im][PF ₆]	[2]	Training	338.15	0.8150	-0.2046	0.3334	1.3957	71.25%	-0.3121	0.7319	10.19%
[C ₄ C ₁ im][PF ₆]	[2]	Training	348.15	1.1020	0.0971	0.6833	1.9805	79.72%	-0.0102	0.9899	10.18%
[C ₄ C ₁ im][PF ₆]	[2]	Training	358.15	1.4400	0.3646	1.0155	2.7608	91.72%	0.2579	1.2942	10.13%
[C ₄ C ₁ im][PF ₆]	[2]	Training	368.15	1.8250	0.6016	1.3313	3.7858	107.44%	0.4973	1.6443	9.90%
[C ₆ C ₁ im][PF ₆]	[2]	Training	278.15	0.0117	-4.4465	-3.1071	0.0447	281.67%	-4.2717	0.0140	19.10%
[C ₆ C ₁ im][PF ₆]	[2]	Training	288.15	0.0270	-3.6104	-2.5902	0.0750	177.40%	-3.5028	0.0301	11.36%
[C ₆ C ₁ im][PF ₆]	[2]	Training	293.15	0.0386	-3.2545	-2.3432	0.0960	148.76%	-3.1587	0.0425	10.05%
[C ₆ C ₁ im][PF ₆]	[2]	Training	303.15	0.0724	-2.6255	-1.8703	0.1541	112.81%	-2.5433	0.0786	8.57%

[C ₆ C ₁ im][PF ₆]	[2]	Training	308.15	0.0964	-2.3392	-1.6438	0.1932	100.46%	-2.2687	0.1034	7.31%
[C ₆ C ₁ im][PF ₆]	[2]	Training	313.15	0.1260	-2.0715	-1.4235	0.2409	91.17%	-2.0141	0.1334	5.91%
[C ₆ C ₁ im][PF ₆]	[2]	Training	318.15	0.1612	-1.8251	-1.2090	0.2985	85.16%	-1.7778	0.1690	4.84%
[C ₆ C ₁ im][PF ₆]	[2]	Training	333.15	0.3069	-1.1812	-0.5988	0.5495	79.04%	-1.1642	0.3122	1.72%
[C ₆ C ₁ im][PF ₆]	[2]	Training	348.15	0.4830	-0.7277	-0.0335	0.9670	100.21%	-0.6663	0.5136	6.34%
[C ₆ C ₁ im][PF ₆]	[2]	Training	328.15	0.2640	-1.3318	-0.7970	0.4507	70.72%	-1.3543	0.2581	2.22%
[C ₃ C ₁ im][SCN]	[2]	Training	323.15	1.3300	0.2852	0.3483	1.4166	6.51%	0.2531	1.2880	3.16%
[C ₃ C ₁ im][SCN]	[2]	Training	318.15	1.1000	0.0953	0.1320	1.1411	3.73%	0.1052	1.1109	0.99%
[C ₃ C ₁ im][SCN]	[2]	Training	313.15	0.9050	-0.0998	-0.0899	0.9140	1.00%	-0.0593	0.9425	4.14%
[C ₃ C ₁ im][SCN]	[2]	Training	308.15	0.7330	-0.3106	-0.3175	0.7280	0.68%	-0.2421	0.7850	7.09%
[C ₃ C ₁ im][SCN]	[2]	Training	303.15	0.5830	-0.5396	-0.5511	0.5763	1.14%	-0.4453	0.6406	9.88%
[C ₃ C ₁ im][SCN]	[2]	Training	298.15	0.4590	-0.7787	-0.7910	0.4534	1.22%	-0.6710	0.5112	11.37%
[C ₃ C ₁ im][SCN]	[2]	Training	293.15	0.3610	-1.0189	-1.0374	0.3544	1.84%	-0.9213	0.3980	10.25%
[C ₂ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	293.15	0.7520	-0.2850	-0.7946	0.4518	39.92%	-0.1777	0.8372	11.33%
[C ₂ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	313.15	1.3500	0.3001	-0.0496	0.9516	29.51%	0.3915	1.4793	9.57%
[C ₂ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	333.15	2.1000	0.7419	0.6077	1.8363	12.56%	0.7959	2.2165	5.55%
[C ₂ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	353.15	3.0500	1.1151	1.1925	3.2952	8.04%	1.0954	2.9903	1.96%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	298.15	0.4030	-0.9088	-1.5611	0.2099	47.91%	-0.9933	0.3704	8.10%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	323.15	0.9100	-0.0943	-0.6168	0.5396	40.70%	-0.1168	0.8897	2.23%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	348.15	1.6200	0.4824	0.2018	1.2236	24.47%	0.4913	1.6345	0.89%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	301.15	0.4525	-0.7930	-1.4401	0.2369	47.65%	-0.8684	0.4196	7.26%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	303.15	0.4876	-0.7183	-1.3607	0.2565	47.40%	-0.7886	0.4545	6.79%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	305.15	0.5244	-0.6455	-1.2823	0.2774	47.10%	-0.7113	0.4910	6.37%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	308.15	0.5812	-0.5427	-1.1664	0.3115	46.41%	-0.6001	0.5487	5.59%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	313.15	0.6839	-0.3799	-0.9778	0.3761	45.00%	-0.4264	0.6529	4.54%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	318.15	0.7955	-0.2288	-0.7947	0.4517	43.22%	-0.2657	0.7666	3.63%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	328.15	1.0750	0.0723	-0.4440	0.6415	40.33%	0.0216	1.0218	4.95%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	333.15	1.2420	0.2167	-0.2759	0.7589	38.90%	0.1506	1.1626	6.39%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	353.15	1.9770	0.6816	0.3528	1.4230	28.02%	0.5920	1.8077	8.57%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	273.15	0.1180	-2.1371	-2.6653	0.0696	41.04%	-2.3254	0.0977	17.17%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	288.15	0.2590	-1.3509	-1.9812	0.1379	46.76%	-1.4587	0.2325	10.22%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	293.15	0.3230	-1.1301	-1.7678	0.1707	47.15%	-1.2160	0.2964	8.23%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	278.15	0.0776	-2.5562	-3.0805	0.0459	40.81%	-2.6641	0.0697	10.23%

[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	288.15	0.1359	-1.9958	-2.6114	0.0734	45.97%	-2.0599	0.1275	6.21%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	298.15	0.2178	-1.5242	-2.1704	0.1141	47.60%	-1.5558	0.2110	3.11%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	308.15	0.3275	-1.1163	-1.7547	0.1730	47.19%	-1.1349	0.3215	1.85%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	318.15	0.4660	-0.7636	-1.3619	0.2562	45.03%	-0.7818	0.4576	1.80%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	328.15	0.6340	-0.4557	-0.9901	0.3715	41.40%	-0.4827	0.6171	2.66%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	338.15	0.8300	-0.1863	-0.6374	0.5287	36.31%	-0.2262	0.7976	3.91%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	348.15	1.0540	0.0526	-0.3023	0.7391	29.88%	-0.0029	0.9971	5.39%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	368.15	1.5790	0.4568	0.3204	1.3777	12.75%	0.3719	1.4504	8.14%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	378.15	1.8750	0.6286	0.6104	1.8411	1.81%	0.5332	1.7043	9.10%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	388.15	2.1920	0.7848	0.8873	2.4285	10.79%	0.6816	1.9771	9.81%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	398.15	2.5260	0.9266	1.1521	3.1649	25.29%	0.8194	2.2691	10.17%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	293.15	0.1700	-1.7720	-2.3876	0.0919	45.97%	-1.7964	0.1659	2.42%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	303.15	0.2700	-1.3093	-1.9595	0.1409	47.80%	-1.3359	0.2629	2.63%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	313.15	0.3900	-0.9416	-1.5555	0.2111	45.88%	-0.9508	0.3864	0.91%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	333.15	0.7200	-0.3285	-0.8115	0.4442	38.30%	-0.3497	0.7049	2.10%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	353.15	1.2000	0.1823	-0.1409	0.8686	27.62%	0.0987	1.1037	8.02%
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	283.15	0.1020	-2.2828	-2.8423	0.0583	42.85%	-2.3485	0.0955	6.36%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	278.15	0.7020	-0.3538	-0.6361	0.5294	24.59%	-0.4616	0.6303	10.22%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	283.15	0.8840	-0.1233	-0.4017	0.6692	24.30%	-0.2233	0.7999	9.52%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	288.15	1.0880	0.0843	-0.1752	0.8393	22.86%	-0.0074	0.9927	8.76%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	298.15	1.5560	0.4421	0.2557	1.2913	17.01%	0.3652	1.4408	7.40%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	303.15	1.8080	0.5922	0.4608	1.5853	12.32%	0.5256	1.6915	6.45%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	313.15	2.3790	0.8667	0.8518	2.3438	1.48%	0.8029	2.2321	6.17%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	323.15	3.0120	1.1026	1.2192	3.3846	12.37%	1.0323	2.8074	6.79%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	333.15	3.6940	1.3067	1.5652	4.7835	29.49%	1.2235	3.3991	7.98%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	343.15	4.4120	1.4843	1.8914	6.6284	50.24%	1.3847	3.9938	9.48%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Training	353.15	5.1000	1.6292	2.1994	9.0197	76.86%	1.5222	4.5824	10.15%
[C ₈ C ₁ im][BF ₄]	[2]	Training	298.15	0.0587	-2.8353	-3.2444	0.0390	33.57%	-2.8122	0.0601	2.34%
[C ₈ C ₁ im][BF ₄]	[2]	Training	348.15	0.4860	-0.7215	-0.8796	0.4150	14.62%	-0.6142	0.5411	11.33%
[C ₈ C ₁ im][BF ₄]	[2]	Training	308.15	0.1012	-2.2907	-2.7262	0.0655	35.31%	-2.2054	0.1102	8.90%
[C ₈ C ₁ im][BF ₄]	[2]	Training	318.15	0.1647	-1.8036	-2.2323	0.1073	34.86%	-1.6967	0.1833	11.29%
[C ₈ C ₁ im][BF ₄]	[2]	Training	328.15	0.2520	-1.3783	-1.7609	0.1719	31.79%	-1.2709	0.2806	11.34%
[C ₈ C ₁ im][BF ₄]	[2]	Training	338.15	0.3680	-0.9997	-1.3105	0.2697	26.71%	-0.9142	0.4008	8.93%

[C ₈ C ₁ im][BF ₄]	[2]	Training	358.15	0.6880	-0.3740	-0.4670	0.6269	8.89%	-0.3604	0.6974	1.37%
[C ₂ C ₁ im][C(CN) ₃]	[2]	Training	298.00	0.7600	-0.2744	0.1550	1.1676	53.64%	-0.3617	0.6965	8.36%
[C ₂ C ₁ im][C(CN) ₃]	[2]	Training	313.00	1.2500	0.2231	0.7832	2.1884	75.08%	0.1180	1.1252	9.98%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	268.15	0.0539	-2.9206	-3.2337	0.0394	26.88%	-3.0282	0.0484	10.20%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	288.15	0.1808	-1.7104	-2.2018	0.1106	38.83%	-1.6806	0.1863	3.02%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	298.15	0.2900	-1.2379	-1.7310	0.1771	38.93%	-1.1654	0.3118	7.52%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	308.15	0.4360	-0.8301	-1.2866	0.2762	36.65%	-0.7347	0.4796	10.01%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	318.15	0.6210	-0.4764	-0.8662	0.4205	32.28%	-0.3738	0.6881	10.81%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	348.15	1.4260	0.3549	0.2699	1.3098	8.15%	0.4123	1.5103	5.91%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	358.15	1.7750	0.5738	0.6121	1.8443	3.90%	0.6063	1.8335	3.30%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	368.15	2.1600	0.7701	0.9381	2.5552	18.30%	0.7771	2.1752	0.70%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	293.15	0.2300	-1.4697	-1.9630	0.1404	38.94%	-1.4114	0.2438	6.00%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	313.15	0.5200	-0.6539	-1.0736	0.3418	34.27%	-0.5464	0.5790	11.35%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	333.15	0.9400	-0.0619	-0.2763	0.7586	19.30%	0.0651	1.0672	13.54%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Training	353.15	1.6000	0.4700	0.4431	1.5575	2.66%	0.5125	1.6694	4.34%
[C ₈ C ₁ im][PF ₆]	[2]	Training	283.15	0.0081	-4.8196	-3.6176	0.0268	232.68%	-4.7177	0.0089	10.73%
[C ₈ C ₁ im][PF ₆]	[2]	Training	288.15	0.0121	-4.4129	-3.3539	0.0349	188.36%	-4.3281	0.0132	8.85%
[C ₈ C ₁ im][PF ₆]	[2]	Training	298.15	0.0252	-3.6809	-2.8483	0.0579	129.92%	-3.6332	0.0264	4.89%
[C ₈ C ₁ im][PF ₆]	[2]	Training	303.15	0.0353	-3.3439	-2.6058	0.0738	109.19%	-3.3245	0.0360	1.95%
[C ₈ C ₁ im][PF ₆]	[2]	Training	308.15	0.0479	-3.0386	-2.3697	0.0935	95.22%	-3.0394	0.0479	0.08%
[C ₈ C ₁ im][PF ₆]	[2]	Training	313.15	0.0653	-2.7288	-2.1397	0.1177	80.23%	-2.7761	0.0623	4.62%
[C ₈ C ₁ im][PF ₆]	[2]	Training	318.15	0.0858	-2.4557	-1.9156	0.1473	71.63%	-2.5327	0.0794	7.41%
[C ₈ C ₁ im][PF ₆]	[2]	Training	323.15	0.1108	-2.2000	-1.6970	0.1832	65.36%	-2.3077	0.0995	10.21%
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	293.15	0.1000	-2.3026	-2.9815	0.0507	49.28%	-2.1951	0.1113	11.34%
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	298.15	0.1300	-2.0402	-2.7545	0.0636	51.05%	-1.9487	0.1425	9.58%
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	303.15	0.1600	-1.8326	-2.5338	0.0794	50.40%	-1.7252	0.1781	11.34%
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	313.15	0.2400	-1.4271	-2.1101	0.1212	49.49%	-1.3382	0.2623	9.30%
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	333.15	0.4700	-0.7550	-1.3263	0.2655	43.52%	-0.7504	0.4722	0.46%
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Training	353.15	0.8000	-0.2231	-0.6161	0.5401	32.49%	-0.3281	0.7203	9.96%
[C ₄ C ₁ im][BF ₄]	[2]	Test	308.20	0.3640	-1.0106	-0.7831	0.4570	25.54%	-0.9327	0.3935	8.10%
[C ₆ C ₁ im][BF ₄]	[2]	Test	308.15	0.2070	-1.5750	-1.8333	0.1599	22.76%	-1.5759	0.2068	0.08%
[C ₄ C ₁ im][CH ₃ CO ₂]	[2]	Test	358.15	0.7360	-0.3065	-0.2546	0.7752	5.33%	-0.2365	0.7894	7.26%
[C ₂ C ₁ im][C ₈ H ₁₇ SO ₄]	[2]	Test	293.10	0.0340	-3.3814	-2.6029	0.0741	117.82%	-3.4519	0.0317	6.81%

[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Test	298.15	0.4550	-0.7875	-1.8019	0.1650	63.74%	-0.9758	0.3769	17.17%
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Test	303.15	0.5470	-0.6033	-1.5685	0.2084	61.91%	-0.7414	0.4764	12.90%
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Test	318.15	0.9200	-0.0834	-0.9045	0.4047	56.01%	-0.1554	0.8561	6.95%
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Test	323.15	1.0500	0.0488	-0.6944	0.4994	52.44%	0.0070	1.0070	4.10%
[C ₄ C ₁ im][CF ₃ CO ₂]	[2]	Test	333.15	1.3800	0.3221	-0.2897	0.7485	45.76%	0.2917	1.3386	3.00%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Test	288.15	0.1420	-1.9519	-1.8586	0.1559	9.78%	-2.0424	0.1297	8.65%
[C ₂ C ₁ im][CH ₃ SO ₃]	[2]	Test	283.15	0.0988	-2.3147	-2.1049	0.1219	23.34%	-2.3822	0.0923	6.54%
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Test	298.15	0.5390	-0.6180	-0.6737	0.5098	5.42%	-0.6508	0.5216	3.22%
[C ₂ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Test	328.15	1.3180	0.2761	0.4427	1.5570	18.13%	0.3465	1.4142	7.30%
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Test	293.15	0.1303	-2.0379	-2.0089	0.1341	2.95%	-2.1716	0.1140	12.52%
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	[2]	Test	323.15	0.4400	-0.8210	-0.7667	0.4645	5.58%	-0.8009	0.4489	2.03%
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Test	308.10	0.6100	-0.4943	-1.2079	0.2988	51.01%	-0.5213	0.5937	2.67%
[C ₂ C ₁ im][C ₂ H ₅ SO ₄]	[2]	Test	308.15	0.5660	-0.5692	-1.2058	0.2994	47.10%	-0.5198	0.5947	5.06%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Test	368.15	1.2930	0.2570	0.7223	2.0592	59.26%	0.1679	1.1828	8.53%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Test	328.15	0.4747	-0.7451	-0.4338	0.6481	36.52%	-0.8506	0.4272	10.01%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Test	313.15	0.2780	-1.2801	-0.9384	0.3913	40.74%	-1.3577	0.2573	7.46%
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	[2]	Test	293.15	0.1122	-2.1875	-1.6873	0.1850	64.90%	-2.2033	0.1104	1.57%
[C ₆ C ₁ im][PF ₆]	[2]	Test	283.15	0.0184	-3.9981	-2.8447	0.0582	216.91%	-3.8734	0.0208	13.29%
[C ₆ C ₁ im][PF ₆]	[2]	Test	298.15	0.0519	-2.9584	-2.1034	0.1220	135.16%	-2.8394	0.0585	12.64%
[C ₆ C ₁ im][PF ₆]	[2]	Test	343.15	0.4510	-0.7963	-0.2173	0.8047	78.42%	-0.8213	0.4398	2.47%
[C ₆ C ₁ im][PF ₆]	[2]	Test	323.15	0.2120	-1.5512	-1.0003	0.3678	73.48%	-1.5584	0.2105	0.72%
[C ₃ C ₁ im][SCN]	[2]	Test	288.15	0.2550	-1.3665	-1.2907	0.2751	7.87%	-1.1986	0.3016	18.29%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Test	283.15	0.2070	-1.5750	-2.2017	0.1106	46.56%	-1.7232	0.1785	13.77%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Test	311.15	0.6429	-0.4418	-1.0526	0.3490	45.71%	-0.4942	0.6100	5.11%
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	[2]	Test	278.15	0.1580	-1.8452	-2.4296	0.0881	44.26%	-2.0115	0.1338	15.32%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Test	273.15	0.5450	-0.6070	-0.8788	0.4153	23.80%	-0.7243	0.4847	11.07%
[C ₂ C ₁ im][B(CN) ₄]	[2]	Test	293.15	1.3110	0.2708	0.0438	1.0448	20.31%	0.1882	1.2071	7.93%
[C ₈ C ₁ im][BF ₄]	[2]	Test	323.15	0.2030	-1.5945	-1.9939	0.1362	32.92%	-1.4743	0.2289	12.77%
[C ₈ C ₁ im][BF ₄]	[2]	Test	288.15	0.0304	-3.4933	-3.7890	0.0226	25.60%	-3.5327	0.0292	3.86%
[C ₂ C ₁ im][C(CN) ₃]	[2]	Test	303.00	0.9300	-0.0726	0.3707	1.4488	55.78%	-0.1873	0.8292	10.84%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Test	278.15	0.1038	-2.2653	-2.7017	0.0671	35.36%	-2.2964	0.1006	3.06%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Test	328.15	0.8480	-0.1649	-0.4678	0.6264	26.13%	-0.0695	0.9329	10.01%
[C ₄ C ₁ im][CF ₃ SO ₃]	[2]	Test	338.15	1.1170	0.1106	-0.0896	0.9143	18.15%	0.1895	1.2087	8.21%

[C ₈ C ₁ im][PF ₆]	[2]	Test	293.15	0.0177	-4.0342	-3.0976	0.0452	155.13%	-3.9671	0.0189	6.93%
[C ₈ C ₁ im][PF ₆]	[2]	Test	348.15	0.2900	-1.2379	-0.6808	0.5062	74.56%	-1.4049	0.2454	15.38%
[C ₄ C ₁ im][CH ₃ SO ₄]	[97]	Test	333.15	0.6230	-0.4732	-1.0645	0.3449	44.64%	-0.2859	0.7514	20.61%
[C ₄ C ₁ im][CH ₃ SO ₄]	[97]	Test	343.15	0.8840	-0.1233	-0.6746	0.5094	42.38%	-0.0501	0.9512	7.60%
[C ₂ C ₁ im][CH ₃ CO ₂]	[98]	Test	338.15	1.4770	0.3900	0.7122	2.0384	38.01%	0.3636	1.4385	2.61%
[C ₂ C ₁ im][CH ₃ CO ₂]	[98]	Test	348.15	1.9560	0.6709	1.0808	2.9469	50.66%	0.6990	2.0118	2.85%
[C ₂ C ₁ im][CH ₃ CO ₂]	[98]	Test	358.15	2.5030	0.9175	1.4323	4.1885	67.34%	0.9875	2.6846	7.26%
[C ₃ C ₁ im][N(CF ₃ SO ₂) ₂]	[99]	Test	283.00	0.3210	-1.1363	-1.8339	0.1598	50.22%	-1.2513	0.2861	10.86%
[C ₃ C ₁ im][N(CF ₃ SO ₂) ₂]	[99]	Test	292.00	0.4770	-0.7402	-1.4517	0.2342	50.91%	-0.8211	0.4399	7.77%
[C ₃ C ₁ im][N(CF ₃ SO ₂) ₂]	[99]	Test	303.00	0.7100	-0.3425	-1.0143	0.3627	48.92%	-0.3770	0.6859	3.39%
[C ₃ C ₁ im][N(CF ₃ SO ₂) ₂]	[99]	Test	313.00	0.9710	-0.0294	-0.6421	0.5262	45.81%	-0.0369	0.9638	0.74%
[C ₃ C ₁ im][N(CF ₃ SO ₂) ₂]	[99]	Test	323.00	1.2520	0.2247	-0.2919	0.7469	40.35%	0.2547	1.2901	3.04%

Table S3. Full name, abbreviation, and numbering of IL cation and anion

No	Name	Abbreviations
Cation		
1	1-propyl-3-methylimidazolium	[C ₃ C ₁ im] ⁺
2	1-butyl-3-methylimidazolium	[C ₄ C ₁ im] ⁺
3	1-pentyl-3-methylimidazolium	[C ₅ C ₁ im] ⁺
4	1-hexyl-3-methylimidazolium	[C ₆ C ₁ im] ⁺
5	1-heptyl-3-methylimidazolium	[C ₇ C ₁ im] ⁺
6	1-octyl-3-methylimidazolium	[C ₈ C ₁ im] ⁺
7	1-nonyl-3-methylimidazolium	[C ₉ C ₁ im] ⁺
Anion		
1	Bis(biphenyldiolato)borate	[BC ₂₄ H ₁₆ O ₄] ⁻
2	Dibutylphosphate	[(C ₄ H ₉ O) ₂ PO ₂] ⁻
3	Tris(nonafluorobutyl)trifluorophosphate	[(C ₄ F ₉) ₃ PF ₃] ⁻
4	Decanoate	[C ₉ H ₂₀ CO ₂] ⁻
5	2-(2-Methoxyethoxy)ethylsulphate	[C ₅ OC ₁ SO ₄] ⁻
6	Octylsulphate	[C ₈ H ₁₇ SO ₄] ⁻
7	Bis(salicylato)borate	[BC ₁₄ H ₈ O ₆] ⁻
8	Diethylphosphate	[(C ₂ H ₅ O) ₂ PO ₂] ⁻
9	Toluene-4-sulfonate(tosylate)	[C ₇ H ₈ SO ₃] ⁻
10	Ethoxyethylsulphate	[C ₄ H ₉ OSO ₄] ⁻
11	Dimethylphosphate	[(CH ₃ O) ₂ PO ₂] ⁻
12	Methoxyethylsulphate	[C ₃ H ₇ OSO ₄] ⁻
13	Benzoate	[(C ₆ H ₅)CO ₂] ⁻
14	Butylsulphate	[C ₄ H ₉ SO ₄] ⁻
15	acetate	[CH ₃ CO ₂] ⁻
16	Methanesulfonate	[CH ₃ SO ₃] ⁻
17	Boron tetrachloride	[BCl ₄] ⁻
18	Ethylsulfate	[C ₂ H ₅ SO ₄] ⁻
19	Hexafluorophosphate	[PF ₆] ⁻
20	Bis(malonato)borate	[C ₆ H ₄ BO ₈] ⁻
21	Tris(pentafluoroethyl)trifluorophosphate	[(C ₂ F ₅) ₃ PF ₃] ⁻
22	Hexafluoroarsenate	[AsF ₆] ⁻
23	Bis(pentafluoroethylsulfonyl)imide	[N(C ₂ F ₅ SO ₂) ₂] ⁻
24	Perchlorate	[ClO ₄] ⁻
25	Salicylate	[C ₇ H ₅ O ₃] ⁻
26	Hexafluorostibate	[SbF ₆] ⁻
27	Tris(trifluoromethylsulfonyl)methide	[C(SO ₂ CF ₃) ₃] ⁻
28	Methylsulphate	[CH ₃ SO ₄] ⁻
29	Tetrafluoroborate	[BF ₄] ⁻
30	Heptafluorobutanoate	[C ₃ F ₇ CO ₂] ⁻
31	Trifluoromethanesulfonate	[CF ₃ SO ₃] ⁻
32	Bis(pentafluoroethyl)phosphinate	[PO ₂ (C ₂ F ₅) ₂] ⁻
33	Trifluoroacetate	[CF ₃ CO ₂] ⁻
34	Thiocyanate	[SCN] ⁻
35	Bis(trifluoromethanesulfonyl)methane	[CH(CF ₃ SO ₂) ₂] ⁻
36	Tricyanomethanide	[C(CN) ₃] ⁻
37	Bis(trifluoromethanesulfonyl)imide	[N(CF ₃ SO ₂) ₂] ⁻
38	Bis(oxalate)borate	[B(C ₂ O ₄) ₂] ⁻
39	Tetracyanoborate	[B(CN) ₄] ⁻
40	Nitrate	[NO ₃] ⁻
41	Nitrite	[NO ₂] ⁻

Table S4. Cation-anion interaction energies and predicted ionic conductivity values for 287 ILs at 298.15 K using SVM regression algorithm

Ionic Liquids	Interaction Energy/ $kcal \cdot mol^{-1}$						$\ln \sigma_{pred}$	$\sigma_{pred}/S \cdot m^{-1}$
	$E_{MF,Cation}$	$E_{MF,Anion}$	$E_{vdW,Cation}$	$E_{vdW,Anion}$	$E_{Diel,Cation}$	$E_{Diel,Anion}$		
[C ₃ C ₁ im][BC ₂₄ H ₁₆ O ₄]	3.5089	6.0956	-9.1931	-18.4872	-50.1735	-67.6201	-12.2912	0.0000
[C ₃ C ₁ im][(C ₄ H ₉ O) ₂ PO ₂]	5.4957	5.9063	-8.8396	-12.8721	-50.1735	-79.8432	-9.0917	0.0001
[C ₃ C ₁ im][(C ₄ F ₉) ₃ PF ₃]	3.2206	5.2683	-7.0746	-15.2128	-50.1735	-40.2288	-8.8575	0.0001
[C ₃ C ₁ im][C ₉ H ₂₀ CO ₂]	6.1401	5.4118	-8.9701	-12.3416	-50.1735	-79.4828	-8.2416	0.0003
[C ₃ C ₁ im][C ₅ OC ₁ SO ₄]	5.2419	6.0631	-8.6876	-10.3107	-50.1735	-82.0186	-8.2235	0.0003
[C ₃ C ₁ im][C ₈ H ₁₇ SO ₄]	4.4809	5.1602	-8.7979	-12.4513	-50.1735	-72.5310	-6.9910	0.0009
[C ₃ C ₁ im][BC ₁₄ H ₈ O ₆]	3.7298	4.6950	-8.8461	-13.2360	-50.1735	-65.6566	-6.2219	0.0020
[C ₃ C ₁ im][(C ₂ H ₅ O) ₂ PO ₂]	6.0903	5.1131	-8.8386	-8.7673	-50.1735	-79.4523	-6.2024	0.0020
[C ₃ C ₁ im][C ₇ H ₈ SO ₃]	5.3906	4.7269	-8.9242	-8.9161	-50.1735	-78.1925	-5.1786	0.0056
[C ₃ C ₁ im][C ₄ H ₉ OSO ₄]	5.1328	4.7923	-8.7296	-8.8624	-50.1735	-77.2128	-5.1602	0.0057
[C ₃ C ₁ im][(CH ₃ O) ₂ PO ₂]	6.5882	4.5114	-8.8782	-6.5559	-50.1735	-79.5814	-4.6282	0.0098
[C ₃ C ₁ im][C ₃ H ₇ OSO ₄]	5.3949	4.5038	-8.7219	-7.8025	-50.1735	-77.0174	-4.3956	0.0123
[C ₃ C ₁ im][(C ₆ H ₅)CO ₂]	6.1670	4.1889	-9.0699	-7.3359	-50.1735	-77.2645	-3.8657	0.0209
[C ₃ C ₁ im][C ₄ H ₉ SO ₄]	4.9753	4.0807	-8.7802	-8.3620	-50.1735	-72.1540	-3.3332	0.0357
[C ₃ C ₁ im][CH ₃ CO ₂]	7.9350	3.8013	-8.9881	-4.1415	-50.1735	-79.6259	-3.0006	0.0498
[C ₃ C ₁ im][CH ₃ SO ₃]	6.9437	3.7995	-8.8547	-4.8251	-50.1735	-76.8542	-2.7914	0.0613
[C ₃ C ₁ im][BCl ₄]	3.1344	2.0498	-10.3361	-8.2480	-50.1735	-53.0390	-2.0834	0.1245
[C ₃ C ₁ im][C ₂ H ₅ SO ₄]	5.4393	3.4380	-8.7795	-6.3398	-50.1735	-72.0671	-2.0404	0.1300
[C ₃ C ₁ im][PF ₆]	3.6555	1.3690	-7.7856	-4.1669	-50.1735	-56.5914	-1.8504	0.1572
[C ₃ C ₁ im][C ₆ H ₄ BO ₈]	4.4590	3.5964	-8.4147	-8.6118	-50.1735	-61.0715	-1.8039	0.1647
[C ₃ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	2.9379	4.5782	-7.2257	-9.3812	-50.1735	-41.7902	-1.7614	0.1718
[C ₃ C ₁ im][AsF ₆]	3.4108	1.5275	-7.7032	-4.3887	-50.1735	-54.8906	-1.7287	0.1775
[C ₃ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	3.2803	3.8793	-7.5722	-9.4708	-50.1735	-50.3323	-1.5851	0.2049
[C ₃ C ₁ im][ClO ₄]	4.6555	1.1361	-8.4254	-3.8316	-50.1735	-61.6899	-1.5843	0.2051
[C ₃ C ₁ im][C ₇ H ₅ O ₃]	4.8624	3.1660	-8.9155	-7.4036	-50.1735	-67.3577	-1.5681	0.2084
[C ₃ C ₁ im][SbF ₆]	3.1260	1.8436	-7.6046	-4.7483	-50.1735	-52.5788	-1.3692	0.2543
[C ₃ C ₁ im][C(SO ₂ CF ₃) ₃]	3.1321	3.7474	-7.6283	-9.5861	-50.1735	-48.5232	-1.3558	0.2577
[C ₃ C ₁ im][CH ₃ SO ₄]	5.7008	2.9406	-8.7713	-5.2800	-50.1735	-71.0882	-1.2868	0.2762
[C ₃ C ₁ im][BF ₄]	4.9236	1.2574	-8.2709	-3.4420	-50.1735	-62.9105	-1.2628	0.2829

[C ₃ C ₁ im][C ₃ F ₇ CO ₂]	4.4913	3.0589	-7.7679	-6.1987	-50.1735	-61.9876	-0.9570	0.3840
[C ₃ C ₁ im][CF ₃ SO ₃]	4.3850	2.1848	-8.0989	-4.9705	-50.1735	-60.9237	-0.8805	0.4146
[C ₃ C ₁ im][PO ₂ (C ₂ F ₅) ₂]	3.6605	3.3519	-7.5193	-7.8049	-50.1735	-54.2051	-0.7710	0.4626
[C ₃ C ₁ im][CF ₃ CO ₂]	5.1474	2.2501	-8.1714	-4.1957	-50.1735	-64.7784	-0.7593	0.4680
[C ₃ C ₁ im][SCN]	5.6806	1.6143	-9.6743	-4.6866	-50.1735	-64.8886	-0.6710	0.5112
[C ₃ C ₁ im][CH(CF ₃ SO ₂) ₂]	3.3328	3.2322	-7.8085	-8.0487	-50.1735	-51.9108	-0.6559	0.5190
[C ₃ C ₁ im][C(CN) ₃]	4.4110	2.3714	-8.7474	-6.3373	-50.1735	-53.5982	-0.5920	0.5532
[C ₃ C ₁ im][N(CF ₃ SO ₂) ₂]	3.3868	3.1711	-7.7797	-7.7290	-50.1735	-52.0438	-0.5628	0.5696
[C ₃ C ₁ im][B(C ₂ O ₄) ₂]	3.6351	2.4468	-8.1815	-6.9787	-50.1735	-51.5885	-0.4751	0.6218
[C ₃ C ₁ im][B(CN) ₄]	3.9421	2.8062	-8.7174	-8.2004	-50.1735	-49.0681	-0.4744	0.6222
[C ₃ C ₁ im][NO ₃]	6.3676	1.8424	-8.6671	-3.1107	-50.1735	-69.3606	-0.1465	0.8637
[C ₃ C ₁ im][NO ₂]	7.5549	2.3345	-8.8198	-2.6832	-50.1735	-74.2878	-0.0463	0.9547
[C ₄ C ₁ im][BC ₂₄ H ₁₆ O ₄]	3.7581	6.0855	-10.1929	-18.4729	-50.0718	-67.6201	-12.6273	0.0000
[C ₄ C ₁ im][(C ₄ H ₉ O) ₂ PO ₂]	5.6273	5.8904	-9.8616	-12.8754	-50.0718	-79.8432	-9.5256	0.0001
[C ₄ C ₁ im][(C ₄ F ₉) ₃ PF ₃]	3.3997	5.1692	-7.9952	-15.2422	-50.0718	-40.2288	-9.0542	0.0001
[C ₄ C ₁ im][C ₉ H ₂₀ CO ₂]	6.2470	5.3839	-9.9952	-12.3451	-50.0718	-79.4828	-8.6360	0.0002
[C ₄ C ₁ im][C ₅ OC ₁ SO ₄]	5.4038	6.0349	-9.7012	-10.3143	-50.0718	-82.0186	-8.6016	0.0002
[C ₄ C ₁ im][C ₈ H ₁₇ SO ₄]	4.6585	5.1585	-9.8194	-12.4551	-50.0718	-72.5310	-7.3872	0.0006
[C ₄ C ₁ im][BC ₁₄ H ₈ O ₆]	3.9787	4.7124	-9.8421	-13.2213	-50.0718	-65.6566	-6.6437	0.0013
[C ₄ C ₁ im][(C ₂ H ₅ O) ₂ PO ₂]	6.1863	5.1023	-9.8538	-8.7682	-50.0718	-79.4523	-6.5105	0.0015
[C ₄ C ₁ im][C ₇ H ₈ SO ₃]	5.5304	4.7308	-9.9304	-8.9105	-50.0718	-78.1925	-5.4956	0.0041
[C ₄ C ₁ im][C ₄ H ₉ OSO ₄]	5.2840	4.7946	-9.7431	-8.8643	-50.0718	-77.2128	-5.4737	0.0042
[C ₄ C ₁ im][(CH ₃ O) ₂ PO ₂]	6.6286	4.5093	-9.8885	-6.5551	-50.0718	-79.5814	-4.8226	0.0080
[C ₄ C ₁ im][C ₃ H ₇ OSO ₄]	5.5218	4.5074	-9.7332	-7.8037	-50.0718	-77.0174	-4.6616	0.0095
[C ₄ C ₁ im][(C ₆ H ₅)CO ₂]	6.2630	4.1999	-10.0732	-7.3276	-50.0718	-77.2645	-4.1220	0.0162
[C ₄ C ₁ im][C ₄ H ₉ SO ₄]	5.1275	4.0996	-9.7958	-8.3637	-50.0718	-72.1540	-3.6565	0.0258
[C ₄ C ₁ im][CH ₃ CO ₂]	7.8517	3.8263	-9.9952	-4.1415	-50.0718	-79.6259	-3.0929	0.0454
[C ₄ C ₁ im][CH ₃ SO ₃]	6.9006	3.8194	-9.8622	-4.8250	-50.0718	-76.8542	-2.9260	0.0536
[C ₄ C ₁ im][BCl ₄]	3.5109	2.1445	-11.3510	-8.2352	-50.0718	-53.0390	-2.5620	0.0771
[C ₄ C ₁ im][C ₂ H ₅ SO ₄]	5.5417	3.4749	-9.7896	-6.3389	-50.0718	-72.0671	-2.2929	0.1010
[C ₄ C ₁ im][PF ₆]	3.9648	1.5395	-8.8151	-4.1862	-50.0718	-56.5914	-2.0046	0.1347
[C ₄ C ₁ im][C ₆ H ₄ BO ₈]	4.6824	3.6658	-9.4128	-8.6111	-50.0718	-61.0715	-2.2688	0.1034
[C ₄ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	3.1953	4.4712	-8.1912	-9.4099	-50.0718	-41.7902	-1.9878	0.1370

[C ₄ C ₁ im][AsF ₆]	3.7548	1.6824	-8.7351	-4.4104	-50.0718	-54.8906	-1.9229	0.1462
[C ₄ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	3.5239	3.8599	-8.5268	-9.4915	-50.0718	-50.3323	-1.9700	0.1395
[C ₄ C ₁ im][ClO ₄]	4.7960	1.2984	-9.4329	-3.8300	-50.0718	-61.6899	-1.7676	0.1707
[C ₄ C ₁ im][C ₇ H ₅ O ₃]	5.0315	3.2098	-9.9175	-7.3953	-50.0718	-67.3577	-1.9103	0.1480
[C ₄ C ₁ im][SbF ₆]	3.4929	1.9553	-8.6361	-4.7726	-50.0718	-52.5788	-1.6571	0.1907
[C ₄ C ₁ im][C(SO ₂ CF ₃) ₃]	3.3906	3.7321	-8.5899	-9.6120	-50.0718	-48.5232	-1.7691	0.1705
[C ₄ C ₁ im][CH ₃ SO ₄]	5.7608	2.9964	-9.7778	-5.2778	-50.0718	-71.0882	-1.5146	0.2199
[C ₄ C ₁ im][BF ₄]	5.0328	1.4217	-9.2839	-3.4506	-50.0718	-62.9105	-1.4387	0.2372
[C ₄ C ₁ im][C ₃ F ₇ CO ₂]	4.6676	3.0675	-8.7675	-6.2190	-50.0718	-61.9876	-1.2449	0.2880
[C ₄ C ₁ im][CF ₃ SO ₃]	4.5758	2.2598	-9.1104	-4.9808	-50.0718	-60.9237	-1.1654	0.3118
[C ₄ C ₁ im][PO ₂ (C ₂ F ₅) ₂]	3.8686	3.3233	-8.5020	-7.8301	-50.0718	-54.2051	-1.1374	0.3207
[C ₄ C ₁ im][CF ₃ CO ₂]	5.2761	2.3257	-9.1882	-4.2060	-50.0718	-64.7784	-0.9758	0.3769
[C ₄ C ₁ im][SCN]	5.7028	1.7478	-10.6730	-4.6747	-50.0718	-64.8886	-0.9965	0.3692
[C ₄ C ₁ im][CH(CF ₃ SO ₂) ₂]	3.5966	3.2416	-8.7932	-8.0701	-50.0718	-51.9108	-1.0930	0.3352
[C ₄ C ₁ im][C(CN) ₃]	4.6117	2.4571	-9.7277	-6.2960	-50.0718	-53.5982	-1.0668	0.3441
[C ₄ C ₁ im][N(CF ₃ SO ₂) ₂]	3.6487	3.1844	-8.7570	-7.7428	-50.0718	-52.0438	-0.9933	0.3704
[C ₄ C ₁ im][B(C ₂ O ₄) ₂]	3.9326	2.5426	-9.1770	-6.9820	-50.0718	-51.5885	-0.9369	0.3918
[C ₄ C ₁ im][B(CN) ₄]	4.1987	2.8737	-9.6851	-8.1279	-50.0718	-49.0681	-1.0323	0.3562
[C ₄ C ₁ im][NO ₃]	6.2984	1.9618	-9.6651	-3.1033	-50.0718	-69.3606	-0.3685	0.6918
[C ₄ C ₁ im][NO ₂]	7.3632	2.4317	-9.8217	-2.6795	-50.0718	-74.2878	-0.2139	0.8075
[C ₅ C ₁ im][BC ₂₄ H ₁₆ O ₄]	3.9846	6.0731	-11.2015	-18.4640	-50.0601	-67.6201	-12.0440	0.0000
[C ₅ C ₁ im][(C ₄ H ₉ O) ₂ PO ₂]	5.7421	5.8610	-10.8870	-12.8787	-50.0601	-79.8432	-9.0830	0.0001
[C ₅ C ₁ im][(C ₄ F ₉) ₃ PF ₃]	3.5767	5.0893	-8.9214	-15.2645	-50.0601	-40.2288	-8.6144	0.0002
[C ₅ C ₁ im][C ₉ H ₂₀ CO ₂]	6.3381	5.3500	-11.0236	-12.3482	-50.0601	-79.4828	-8.1976	0.0003
[C ₅ C ₁ im][C ₅ OC ₁ SO ₄]	5.5471	6.0008	-10.7197	-10.3185	-50.0601	-82.0186	-8.2330	0.0003
[C ₅ C ₁ im][C ₈ H ₁₇ SO ₄]	4.8168	5.1459	-10.8443	-12.4590	-50.0601	-72.5310	-7.0317	0.0009
[C ₅ C ₁ im][BC ₁₄ H ₈ O ₆]	4.2001	4.7243	-10.8467	-13.2113	-50.0601	-65.6566	-6.3769	0.0017
[C ₅ C ₁ im][(C ₂ H ₅ O) ₂ PO ₂]	6.2680	5.0810	-10.8745	-8.7692	-50.0601	-79.4523	-6.1877	0.0021
[C ₅ C ₁ im][C ₇ H ₈ SO ₃]	5.6525	4.7271	-10.9444	-8.9070	-50.0601	-78.1925	-5.2495	0.0053
[C ₅ C ₁ im][C ₄ H ₉ OSO ₄]	5.4179	4.7890	-10.7622	-8.8667	-50.0601	-77.2128	-5.2356	0.0053
[C ₅ C ₁ im][(CH ₃ O) ₂ PO ₂]	6.6653	4.4991	-10.9062	-6.5546	-50.0601	-79.5814	-4.5628	0.0104
[C ₅ C ₁ im][C ₃ H ₇ OSO ₄]	5.6359	4.5055	-10.7508	-7.8055	-50.0601	-77.0174	-4.4637	0.0115
[C ₅ C ₁ im][(C ₆ H ₅)CO ₂]	6.3461	4.2056	-11.0859	-7.3217	-50.0601	-77.2645	-3.9380	0.0195

[C ₅ C ₁ im][C ₄ H ₉ SO ₄]	5.2612	4.1088	-10.8169	-8.3656	-50.0601	-72.1540	-3.5553	0.0286
[C ₅ C ₁ im][CH ₃ CO ₂]	7.7889	3.8418	-11.0118	-4.1414	-50.0601	-79.6259	-2.8892	0.0556
[C ₅ C ₁ im][CH ₃ SO ₃]	6.8759	3.8316	-10.8786	-4.8252	-50.0601	-76.8542	-2.7831	0.0618
[C ₅ C ₁ im][BCl ₄]	3.8309	2.2338	-12.3727	-8.2259	-50.0601	-53.0390	-2.9732	0.0511
[C ₅ C ₁ im][C ₂ H ₅ SO ₄]	5.6355	3.5025	-10.8071	-6.3386	-50.0601	-72.0671	-2.2981	0.1004
[C ₅ C ₁ im][PF ₆]	4.2324	1.6872	-9.8445	-4.1986	-50.0601	-56.5914	-2.3854	0.0921
[C ₅ C ₁ im][C ₆ H ₄ BO ₈]	4.8810	3.7262	-10.4185	-8.6124	-50.0601	-61.0715	-2.4062	0.0902
[C ₅ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	3.4366	4.3895	-9.1617	-9.4309	-50.0601	-41.7902	-2.0261	0.1318
[C ₅ C ₁ im][AsF ₆]	4.0491	1.8186	-9.7656	-4.4243	-50.0601	-54.8906	-2.3394	0.0964
[C ₅ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	3.7465	3.8452	-9.4918	-9.5100	-50.0601	-50.3323	-2.1010	0.1223
[C ₅ C ₁ im][ClO ₄]	4.9355	1.4380	-10.4495	-3.8286	-50.0601	-61.6899	-2.1165	0.1205
[C ₅ C ₁ im][C ₇ H ₅ O ₃]	5.1787	3.2457	-10.9288	-7.3898	-50.0601	-67.3577	-2.0140	0.1335
[C ₅ C ₁ im][SbF ₆]	3.8059	2.0589	-9.6655	-4.7885	-50.0601	-52.5788	-2.1442	0.1172
[C ₅ C ₁ im][C(SO ₂ CF ₃) ₃]	3.6267	3.7222	-9.5597	-9.6336	-50.0601	-48.5232	-1.9490	0.1424
[C ₅ C ₁ im][CH ₃ SO ₄]	5.8237	3.0427	-10.7931	-5.2764	-50.0601	-71.0882	-1.6008	0.2017
[C ₅ C ₁ im][BF ₄]	5.1472	1.5626	-10.3040	-3.4558	-50.0601	-62.9105	-1.7725	0.1699
[C ₅ C ₁ im][C ₃ F ₇ CO ₂]	4.8217	3.0755	-9.7712	-6.2343	-50.0601	-61.9876	-1.4450	0.2358
[C ₅ C ₁ im][CF ₃ SO ₃]	4.7430	2.3245	-10.1267	-4.9882	-50.0601	-60.9237	-1.5129	0.2203
[C ₅ C ₁ im][PO ₂ (C ₂ F ₅) ₂]	4.0565	3.3025	-9.4895	-7.8493	-50.0601	-54.2051	-1.3830	0.2508
[C ₅ C ₁ im][CF ₃ CO ₂]	5.3897	2.3889	-10.2095	-4.2135	-50.0601	-64.7784	-1.2341	0.2911
[C ₅ C ₁ im][SCN]	5.7477	1.8611	-11.6897	-4.6716	-50.0601	-64.8886	-1.3301	0.2644
[C ₅ C ₁ im][CH(CF ₃ SO ₂) ₂]	3.8324	3.2535	-9.7846	-8.0873	-50.0601	-51.9108	-1.4146	0.2430
[C ₅ C ₁ im][C(CN) ₃]	4.7856	2.5285	-10.7368	-6.2753	-50.0601	-53.5982	-1.5241	0.2178
[C ₅ C ₁ im][N(CF ₃ SO ₂) ₂]	3.8824	3.1985	-9.7437	-7.7553	-50.0601	-52.0438	-1.3318	0.2640
[C ₅ C ₁ im][B(C ₂ O ₄) ₂]	4.1906	2.6271	-10.1806	-6.9861	-50.0601	-51.5885	-1.3836	0.2507
[C ₅ C ₁ im][B(CN) ₄]	4.4182	2.9307	-10.6864	-8.0836	-50.0601	-49.0681	-1.4655	0.2310
[C ₅ C ₁ im][NO ₃]	6.2686	2.0603	-10.6753	-3.0973	-50.0601	-69.3606	-0.6154	0.5404
[C ₅ C ₁ im][NO ₂]	7.2332	2.5093	-10.8373	-2.6784	-50.0601	-74.2878	-0.3190	0.7268
[C ₆ C ₁ im][BC ₂₄ H ₁₆ O ₄]	4.1951	6.0601	-12.2078	-18.4550	-50.1150	-67.6201	-10.8528	0.0000
[C ₆ C ₁ im][(C ₄ H ₉ O) ₂ PO ₂]	5.8520	5.8366	-11.9098	-12.8825	-50.1150	-79.8432	-8.0903	0.0003
[C ₆ C ₁ im][(C ₄ F ₉) ₃ PF ₃]	3.7433	5.0151	-9.8537	-15.2876	-50.1150	-40.2288	-7.7032	0.0005
[C ₆ C ₁ im][C ₉ H ₂₀ CO ₂]	6.4268	5.3238	-12.0488	-12.3513	-50.1150	-79.4828	-7.2477	0.0007
[C ₆ C ₁ im][C ₅ OC ₁ SO ₄]	5.6872	5.9756	-11.7366	-10.3232	-50.1150	-82.0186	-7.3919	0.0006

[C ₆ C ₁ im][C ₈ H ₁₇ SO ₄]	4.9659	5.1351	-11.8668	-12.4632	-50.1150	-72.5310	-6.1922	0.0020
[C ₆ C ₁ im][BC ₁₄ H ₈ O ₆]	4.4039	4.7342	-11.8503	-13.2023	-50.1150	-65.6566	-5.6398	0.0036
[C ₆ C ₁ im][(C ₂ H ₅ O) ₂ PO ₂]	6.3509	5.0675	-11.8937	-8.7707	-50.1150	-79.4523	-5.4882	0.0041
[C ₆ C ₁ im][C ₇ H ₈ SO ₃]	5.7717	4.7285	-11.9574	-8.9039	-50.1150	-78.1925	-4.6535	0.0095
[C ₆ C ₁ im][C ₄ H ₉ OSO ₄]	5.5491	4.7885	-11.7798	-8.8694	-50.1150	-77.2128	-4.6490	0.0096
[C ₆ C ₁ im][(CH ₃ O) ₂ PO ₂]	6.7135	4.4980	-11.9232	-6.5544	-50.1150	-79.5814	-4.0477	0.0175
[C ₆ C ₁ im][C ₃ H ₇ OSO ₄]	5.7525	4.5106	-11.7674	-7.8077	-50.1150	-77.0174	-3.9767	0.0187
[C ₆ C ₁ im][(C ₆ H ₅)CO ₂]	6.4322	4.2157	-12.0975	-7.3159	-50.1150	-77.2645	-3.4876	0.0306
[C ₆ C ₁ im][C ₄ H ₉ SO ₄]	5.3908	4.1204	-11.8364	-8.3677	-50.1150	-72.1540	-3.1782	0.0417
[C ₆ C ₁ im][CH ₃ CO ₂]	7.7576	3.8632	-12.0278	-4.1410	-50.1150	-79.6259	-2.5403	0.0788
[C ₆ C ₁ im][CH ₃ SO ₃]	6.8801	3.8528	-11.8950	-4.8253	-50.1150	-76.8542	-2.4965	0.0824
[C ₆ C ₁ im][BCl ₄]	4.1149	2.3085	-13.3930	-8.2172	-50.1150	-53.0390	-3.2810	0.0376
[C ₆ C ₁ im][C ₂ H ₅ SO ₄]	5.7349	3.5326	-11.8241	-6.3385	-50.1150	-72.0671	-2.1392	0.1178
[C ₆ C ₁ im][PF ₆]	4.4769	1.8112	-10.8737	-4.2109	-50.1150	-56.5914	-2.8394	0.0585
[C ₆ C ₁ im][C ₆ H ₄ BO ₈]	5.0703	3.7842	-11.4244	-8.6147	-50.1150	-61.0715	-2.2873	0.1015
[C ₆ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	3.6582	4.3155	-10.1368	-9.4516	-50.1150	-41.7902	-1.8997	0.1496
[C ₆ C ₁ im][AsF ₆]	4.3138	1.9322	-10.7952	-4.4378	-50.1150	-54.8906	-2.8260	0.0592
[C ₆ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	3.9525	3.8321	-10.4599	-9.5265	-50.1150	-50.3323	-2.0176	0.1330
[C ₆ C ₁ im][ClO ₄]	5.0831	1.5610	-11.4672	-3.8275	-50.1150	-61.6899	-2.5098	0.0813
[C ₆ C ₁ im][C ₇ H ₅ O ₃]	5.3188	3.2800	-11.9394	-7.3846	-50.1150	-67.3577	-1.9403	0.1437
[C ₆ C ₁ im][SbF ₆]	4.0841	2.1450	-10.6938	-4.8035	-50.1150	-52.5788	-2.6900	0.0679
[C ₆ C ₁ im][C(SO ₂ CF ₃) ₃]	3.8439	3.7125	-10.5332	-9.6540	-50.1150	-48.5232	-1.9246	0.1459
[C ₆ C ₁ im][CH ₃ SO ₄]	5.9015	3.0908	-11.8085	-5.2753	-50.1150	-71.0882	-1.5849	0.2050
[C ₆ C ₁ im][BF ₄]	5.2747	1.6870	-11.3270	-3.4625	-50.1150	-62.9105	-2.1500	0.1165
[C ₆ C ₁ im][C ₃ F ₇ CO ₂]	4.9647	3.0859	-10.7752	-6.2483	-50.1150	-61.9876	-1.5537	0.2115
[C ₆ C ₁ im][CF ₃ SO ₃]	4.9012	2.3832	-11.1424	-4.9948	-50.1150	-60.9237	-1.8489	0.1574
[C ₆ C ₁ im][PO ₂ (C ₂ F ₅) ₂]	4.2290	3.2860	-10.4790	-7.8672	-50.1150	-54.2051	-1.5111	0.2207
[C ₆ C ₁ im][CF ₃ CO ₂]	5.5027	2.4464	-11.2300	-4.2203	-50.1150	-64.7784	-1.4807	0.2275
[C ₆ C ₁ im][SCN]	5.8223	1.9649	-12.6986	-4.6601	-50.1150	-64.8886	-1.6235	0.1972
[C ₆ C ₁ im][CH(CF ₃ SO ₂) ₂]	4.0481	3.2642	-10.7777	-8.1034	-50.1150	-51.9108	-1.6067	0.2006
[C ₆ C ₁ im][C(CN) ₃]	4.9524	2.5923	-11.7357	-6.2437	-50.1150	-53.5982	-1.9075	0.1484
[C ₆ C ₁ im][N(CF ₃ SO ₂) ₂]	4.0968	3.2114	-10.7316	-7.7659	-50.1150	-52.0438	-1.5558	0.2110
[C ₆ C ₁ im][B(C ₂ O ₄) ₂]	4.4259	2.7009	-11.1848	-6.9906	-50.1150	-51.5885	-1.7487	0.1740

[C ₆ C ₁ im][B(CN) ₄]	4.6213	2.9803	-11.6784	-8.0308	-50.1150	-49.0681	-1.7547	0.1730
[C ₆ C ₁ im][NO ₃]	6.2788	2.1515	-11.6871	-3.0917	-50.1150	-69.3606	-0.8581	0.4240
[C ₆ C ₁ im][NO ₂]	7.1636	2.5847	-11.8493	-2.6725	-50.1150	-74.2878	-0.3979	0.6717
[C ₇ C ₁ im][BC ₂₄ H ₁₆ O ₄]	4.3934	6.0479	-13.2275	-18.4470	-50.1751	-67.6201	-9.6649	0.0001
[C ₇ C ₁ im][[(C ₄ H ₉ O) ₂ PO ₂]	5.9601	5.8208	-12.9443	-12.8854	-50.1751	-79.8432	-7.1317	0.0008
[C ₇ C ₁ im][[(C ₄ F ₉) ₃ PF ₃]	3.9027	4.9449	-10.8013	-15.3085	-50.1751	-40.2288	-6.7920	0.0011
[C ₇ C ₁ im][C ₉ H ₂₀ CO ₂]	6.5074	5.2979	-13.0858	-12.3538	-50.1751	-79.4828	-6.3298	0.0018
[C ₇ C ₁ im][C ₅ OC ₁ SO ₄]	5.8318	5.9692	-12.7653	-10.3272	-50.1751	-82.0186	-6.5971	0.0014
[C ₇ C ₁ im][C ₈ H ₁₇ SO ₄]	5.1132	5.1340	-12.9007	-12.4666	-50.1751	-72.5310	-5.4010	0.0045
[C ₇ C ₁ im][BC ₁₄ H ₈ O ₆]	4.5974	4.7477	-12.8676	-13.1940	-50.1751	-65.6566	-4.9350	0.0072
[C ₇ C ₁ im][[(C ₂ H ₅ O) ₂ PO ₂]	6.4369	5.0639	-12.9250	-8.7716	-50.1751	-79.4523	-4.8432	0.0079
[C ₇ C ₁ im][C ₇ H ₈ SO ₃]	5.8930	4.7404	-12.9834	-8.9007	-50.1751	-78.1925	-4.1114	0.0164
[C ₇ C ₁ im][C ₄ H ₉ OSO ₄]	5.6848	4.8026	-12.8095	-8.8716	-50.1751	-77.2128	-4.1181	0.0163
[C ₇ C ₁ im][[(CH ₃ O) ₂ PO ₂]	6.7717	4.5072	-12.9530	-6.5539	-50.1751	-79.5814	-3.5962	0.0274
[C ₇ C ₁ im][C ₃ H ₇ OSO ₄]	5.8767	4.5314	-12.7963	-7.8093	-50.1751	-77.0174	-3.5482	0.0288
[C ₇ C ₁ im][[(C ₆ H ₅)CO ₂]	6.5148	4.2261	-13.1230	-7.3104	-50.1751	-77.2645	-3.0832	0.0458
[C ₇ C ₁ im][C ₄ H ₉ SO ₄]	5.5228	4.1424	-12.8679	-8.3692	-50.1751	-72.1540	-2.8509	0.0578
[C ₇ C ₁ im][CH ₃ CO ₂]	7.7417	3.8842	-13.0575	-4.1404	-50.1751	-79.6259	-2.2516	0.1052
[C ₇ C ₁ im][CH ₃ SO ₃]	6.9081	3.8869	-12.9243	-4.8251	-50.1751	-76.8542	-2.2808	0.1022
[C ₇ C ₁ im][BCl ₄]	4.3789	2.3796	-14.4265	-8.2095	-50.1751	-53.0390	-3.5609	0.0284
[C ₇ C ₁ im][C ₂ H ₅ SO ₄]	5.8437	3.5735	-12.8536	-6.3381	-50.1751	-72.0671	-2.0224	0.1323
[C ₇ C ₁ im][PF ₆]	4.7109	1.9278	-11.9142	-4.2213	-50.1751	-56.5914	-3.2473	0.0389
[C ₇ C ₁ im][C ₆ H ₄ BO ₈]	5.2579	3.8501	-12.4437	-8.6171	-50.1751	-61.0715	-2.1856	0.1124
[C ₇ C ₁ im][[(C ₂ F ₅) ₃ PF ₃]	3.8671	4.2481	-11.1266	-9.4699	-50.1751	-41.7902	-1.8441	0.1582
[C ₇ C ₁ im][AsF ₆]	4.5635	2.0383	-11.8360	-4.4492	-50.1751	-54.8906	-3.2678	0.0381
[C ₇ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	4.1481	3.8229	-11.4435	-9.5415	-50.1751	-50.3323	-1.9655	0.1401
[C ₇ C ₁ im][ClO ₄]	5.2399	1.6817	-12.4980	-3.8263	-50.1751	-61.6899	-2.8565	0.0575
[C ₇ C ₁ im][C ₇ H ₅ O ₃]	5.4521	3.3132	-12.9637	-7.3798	-50.1751	-67.3577	-1.8939	0.1505
[C ₇ C ₁ im][SbF ₆]	4.3435	2.2263	-11.7331	-4.8162	-50.1751	-52.5788	-3.1954	0.0410
[C ₇ C ₁ im][C(SO ₂ CF ₃) ₃]	4.0501	3.7073	-11.5219	-9.6724	-50.1751	-48.5232	-1.9297	0.1452
[C ₇ C ₁ im][CH ₃ SO ₄]	5.9944	3.1486	-12.8369	-5.2740	-50.1751	-71.0882	-1.6005	0.2018
[C ₇ C ₁ im][BF ₄]	5.4154	1.8100	-12.3626	-3.4683	-50.1751	-62.9105	-2.4857	0.0833
[C ₇ C ₁ im][C ₃ F ₇ CO ₂]	5.0983	3.0945	-11.7922	-6.2604	-50.1751	-61.9876	-1.6841	0.1856

[C ₇ C ₁ im][CF ₃ SO ₃]	5.0563	2.4421	-12.1706	-5.0003	-50.1751	-60.9237	-2.1734	0.1138
[C ₇ C ₁ im][PO ₂ (C ₂ F ₅) ₂]	4.3886	3.2688	-11.4823	-7.8828	-50.1751	-54.2051	-1.6733	0.1876
[C ₇ C ₁ im][CF ₃ CO ₂]	5.6138	2.4987	-12.2628	-4.2261	-50.1751	-64.7784	-1.7332	0.1767
[C ₇ C ₁ im][SCN]	5.9135	2.0650	-13.7226	-4.6496	-50.1751	-64.8886	-1.9052	0.1488
[C ₇ C ₁ im][CH(CF ₃ SO ₂) ₂]	4.2519	3.2780	-11.7849	-8.1176	-50.1751	-51.9108	-1.8139	0.1630
[C ₇ C ₁ im][C(CN) ₃]	5.1137	2.6529	-12.7513	-6.2170	-50.1751	-53.5982	-2.2853	0.1017
[C ₇ C ₁ im][N(CF ₃ SO ₂) ₂]	4.3001	3.2276	-11.7342	-7.7753	-50.1751	-52.0438	-1.7934	0.1664
[C ₇ C ₁ im][B(C ₂ O ₄) ₂]	4.6501	2.7757	-12.2029	-6.9950	-50.1751	-51.5885	-2.0941	0.1232
[C ₇ C ₁ im][B(CN) ₄]	4.8139	3.0280	-12.6881	-7.9849	-50.1751	-49.0681	-2.0545	0.1282
[C ₇ C ₁ im][NO ₃]	6.3178	2.2436	-12.7128	-3.0863	-50.1751	-69.3606	-1.1050	0.3312
[C ₇ C ₁ im][NO ₂]	7.1329	2.6606	-12.8756	-2.6676	-50.1751	-74.2878	-0.5191	0.5950
[C ₈ C ₁ im][BC ₂₄ H ₁₆ O ₄]	4.5857	6.0407	-14.2395	-18.4403	-50.2776	-67.6201	-8.2193	0.0003
[C ₈ C ₁ im][(C ₄ H ₉ O) ₂ PO ₂]	6.0761	5.8089	-13.9693	-12.8884	-50.2776	-79.8432	-5.9565	0.0026
[C ₈ C ₁ im][(C ₄ F ₉) ₃ PF ₃]	4.0571	4.8827	-11.7435	-15.3263	-50.2776	-40.2288	-5.6385	0.0036
[C ₈ C ₁ im][C ₉ H ₂₀ CO ₂]	6.6023	5.2855	-14.1134	-12.3562	-50.2776	-79.4828	-5.2410	0.0053
[C ₈ C ₁ im][C ₅ OC ₁ SO ₄]	5.9782	5.9623	-13.7851	-10.3314	-50.2776	-82.0186	-5.5990	0.0037
[C ₈ C ₁ im][C ₈ H ₁₇ SO ₄]	5.2611	5.1320	-13.9252	-12.4702	-50.2776	-72.5310	-4.4157	0.0121
[C ₈ C ₁ im][BC ₁₄ H ₈ O ₆]	4.7846	4.7616	-13.8775	-13.1872	-50.2776	-65.6566	-4.0346	0.0177
[C ₈ C ₁ im][(C ₂ H ₅ O) ₂ PO ₂]	6.5343	5.0633	-13.9478	-8.7727	-50.2776	-79.4523	-4.0658	0.0171
[C ₈ C ₁ im][C ₇ H ₈ SO ₃]	6.0202	4.7530	-14.0015	-8.8982	-50.2776	-78.1925	-3.4414	0.0320
[C ₈ C ₁ im][C ₄ H ₉ OSO ₄]	5.8232	4.8140	-13.8305	-8.8740	-50.2776	-77.2128	-3.4473	0.0318
[C ₈ C ₁ im][(CH ₃ O) ₂ PO ₂]	6.8470	4.5187	-13.9749	-6.5537	-50.2776	-79.5814	-3.0695	0.0464
[C ₈ C ₁ im][C ₃ H ₇ OSO ₄]	6.0063	4.5496	-13.8167	-7.8112	-50.2776	-77.0174	-3.0057	0.0495
[C ₈ C ₁ im][(C ₆ H ₅)CO ₂]	6.6128	4.2444	-14.1409	-7.3056	-50.2776	-77.2645	-2.6116	0.0734
[C ₈ C ₁ im][C ₄ H ₉ SO ₄]	5.6577	4.1613	-13.8907	-8.3709	-50.2776	-72.1540	-2.4170	0.0892
[C ₈ C ₁ im][CH ₃ CO ₂]	7.7600	3.9103	-14.0798	-4.1398	-50.2776	-79.6259	-1.9597	0.1409
[C ₈ C ₁ im][CH ₃ SO ₃]	6.9605	3.9183	-13.9461	-4.8250	-50.2776	-76.8542	-2.0293	0.1314
[C ₈ C ₁ im][BCl ₄]	4.6184	2.4390	-15.4515	-8.2030	-50.2776	-53.0390	-3.7643	0.0232
[C ₈ C ₁ im][C ₂ H ₅ SO ₄]	5.9602	3.6093	-13.8750	-6.3381	-50.2776	-72.0671	-1.8440	0.1582
[C ₈ C ₁ im][PF ₆]	4.9272	2.0251	-12.9438	-4.2293	-50.2776	-56.5914	-3.6332	0.0264
[C ₈ C ₁ im][C ₆ H ₄ BO ₈]	5.4403	3.9089	-13.4553	-8.6203	-50.2776	-61.0715	-1.9519	0.1420
[C ₈ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	4.0632	4.1887	-12.1095	-9.4850	-50.2776	-41.7902	-1.7114	0.1806
[C ₈ C ₁ im][AsF ₆]	4.7920	2.1266	-12.8656	-4.4579	-50.2776	-54.8906	-3.6812	0.0252

[C ₈ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	4.3339	3.8142	-12.4226	-9.5556	-50.2776	-50.3323	-1.7975	0.1657
[C ₈ C ₁ im][ClO ₄]	5.3964	1.7844	-13.5208	-3.8253	-50.2776	-61.6899	-3.1914	0.0411
[C ₈ C ₁ im][C ₇ H ₅ O ₃]	5.5900	3.3479	-13.9804	-7.3759	-50.2776	-67.3577	-1.7796	0.1687
[C ₈ C ₁ im][SbF ₆]	4.5796	2.2938	-12.7613	-4.8260	-50.2776	-52.5788	-3.6625	0.0257
[C ₈ C ₁ im][C(SO ₂ CF ₃) ₃]	4.2447	3.7017	-12.5047	-9.6890	-50.2776	-48.5232	-1.8193	0.1621
[C ₈ C ₁ im][CH ₃ SO ₄]	6.0991	3.1996	-13.8577	-5.2732	-50.2776	-71.0882	-1.5774	0.2065
[C ₈ C ₁ im][BF ₄]	5.5598	1.9144	-13.3892	-3.4725	-50.2776	-62.9105	-2.8122	0.0601
[C ₈ C ₁ im][C ₃ F ₇ CO ₂]	5.2351	3.1086	-12.8011	-6.2709	-50.2776	-61.9876	-1.7620	0.1717
[C ₈ C ₁ im][CF ₃ SO ₃]	5.2095	2.4943	-13.1902	-5.0049	-50.2776	-60.9237	-2.4614	0.0853
[C ₈ C ₁ im][PO ₂ (C ₂ F ₅) ₂]	4.5463	3.2596	-12.4783	-7.8962	-50.2776	-54.2051	-1.7643	0.1713
[C ₈ C ₁ im][CF ₃ CO ₂]	5.7328	2.5484	-13.2866	-4.2310	-50.2776	-64.7784	-1.9655	0.1401
[C ₈ C ₁ im][SCN]	6.0178	2.1523	-14.7437	-4.6451	-50.2776	-64.8886	-2.1675	0.1145
[C ₈ C ₁ im][CH(CF ₃ SO ₂) ₂]	4.4449	3.2904	-12.7850	-8.1301	-50.2776	-51.9108	-1.9319	0.1449
[C ₈ C ₁ im][C(CN) ₃]	5.2701	2.7055	-13.7675	-6.1994	-50.2776	-53.5982	-2.6055	0.0739
[C ₈ C ₁ im][N(CF ₃ SO ₂) ₂]	4.4918	3.2412	-12.7311	-7.7845	-50.2776	-52.0438	-1.9487	0.1425
[C ₈ C ₁ im][B(C ₂ O ₄) ₂]	4.8596	2.8400	-13.2137	-7.0000	-50.2776	-51.5885	-2.3574	0.0947
[C ₈ C ₁ im][B(CN) ₄]	4.9953	3.0686	-13.6990	-7.9502	-50.2776	-49.0681	-2.2728	0.1030
[C ₈ C ₁ im][NO ₃]	6.3821	2.3238	-13.7317	-3.0816	-50.2776	-69.3606	-1.3510	0.2590
[C ₈ C ₁ im][NO ₂]	7.1421	2.7282	-13.8964	-2.6642	-50.2776	-74.2878	-0.6541	0.5199
[C ₉ C ₁ im][BC ₂₄ H ₁₆ O ₄]	4.7670	6.0331	-15.2694	-18.4336	-50.3203	-67.6201	-7.4356	0.0006
[C ₉ C ₁ im][(C ₄ H ₉ O) ₂ PO ₂]	6.1731	5.7974	-15.0115	-12.8911	-50.3203	-79.8432	-5.3960	0.0045
[C ₉ C ₁ im][(C ₄ F ₉) ₃ PF ₃]	4.1984	4.8161	-12.7078	-15.3442	-50.3203	-40.2288	-5.0430	0.0065
[C ₉ C ₁ im][C ₉ H ₂₀ CO ₂]	6.6756	5.2677	-15.1572	-12.3581	-50.3203	-79.4828	-4.7349	0.0088
[C ₉ C ₁ im][C ₅ OC ₁ SO ₄]	6.1134	5.9652	-14.8231	-10.3352	-50.3203	-82.0186	-5.1541	0.0058
[C ₉ C ₁ im][C ₈ H ₁₇ SO ₄]	5.3934	5.1327	-14.9671	-12.4733	-50.3203	-72.5310	-4.0068	0.0182
[C ₉ C ₁ im][BC ₁₄ H ₈ O ₆]	4.9577	4.7754	-14.9061	-13.1808	-50.3203	-65.6566	-3.6895	0.0250
[C ₉ C ₁ im][(C ₂ H ₅ O) ₂ PO ₂]	6.6142	5.0662	-14.9883	-8.7736	-50.3203	-79.4523	-3.7557	0.0234
[C ₉ C ₁ im][C ₇ H ₈ SO ₃]	6.1315	4.7693	-15.0379	-8.8958	-50.3203	-78.1925	-3.2127	0.0402
[C ₉ C ₁ im][C ₄ H ₉ OSO ₄]	5.9497	4.8327	-14.8696	-8.8761	-50.3203	-77.2128	-3.2207	0.0399
[C ₉ C ₁ im][(CH ₃ O) ₂ PO ₂]	6.9074	4.5348	-15.0146	-6.5535	-50.3203	-79.5814	-2.9034	0.0548
[C ₉ C ₁ im][C ₃ H ₇ OSO ₄]	6.1254	4.5760	-14.8554	-7.8129	-50.3203	-77.0174	-2.8526	0.0577
[C ₉ C ₁ im][(C ₆ H ₅)CO ₂]	6.6943	4.2611	-15.1766	-7.3010	-50.3203	-77.2645	-2.4946	0.0825
[C ₉ C ₁ im][C ₄ H ₉ SO ₄]	5.7787	4.1846	-14.9313	-8.3723	-50.3203	-72.1540	-2.3499	0.0954

[C ₉ C ₁ im][CH ₃ CO ₂]	7.7639	3.9363	-15.1197	-4.1390	-50.3203	-79.6259	-1.9221	0.1463
[C ₉ C ₁ im][CH ₃ SO ₃]	7.0034	3.9568	-14.9862	-4.8248	-50.3203	-76.8542	-2.0359	0.1306
[C ₉ C ₁ im][BCl ₄]	4.8415	2.4951	-16.4945	-8.1968	-50.3203	-53.0390	-4.0656	0.0172
[C ₉ C ₁ im][C ₂ H ₅ SO ₄]	6.0657	3.6506	-14.9147	-6.3379	-50.3203	-72.0671	-1.9113	0.1479
[C ₉ C ₁ im][PF ₆]	5.1303	2.1180	-13.9924	-4.2375	-50.3203	-56.5914	-3.9470	0.0193
[C ₉ C ₁ im][C ₆ H ₄ BO ₈]	5.6128	3.9709	-14.4862	-8.6234	-50.3203	-61.0715	-2.0337	0.1309
[C ₉ C ₁ im][(C ₂ F ₅) ₃ PF ₃]	4.2438	4.1279	-13.1137	-9.4998	-50.3203	-41.7902	-1.9115	0.1479
[C ₉ C ₁ im][AsF ₆]	5.0057	2.2103	-13.9141	-4.4668	-50.3203	-54.8906	-4.0274	0.0178
[C ₉ C ₁ im][N(C ₂ F ₅ SO ₂) ₂]	4.5074	3.8059	-13.4217	-9.5679	-50.3203	-50.3323	-1.9424	0.1434
[C ₉ C ₁ im][ClO ₄]	5.5468	1.8860	-14.5623	-3.8244	-50.3203	-61.6899	-3.4612	0.0314
[C ₉ C ₁ im][C ₇ H ₅ O ₃]	5.7134	3.3818	-15.0154	-7.3722	-50.3203	-67.3577	-1.9073	0.1485
[C ₉ C ₁ im][SbF ₆]	4.7991	2.3575	-13.8083	-4.8358	-50.3203	-52.5788	-4.0749	0.0170
[C ₉ C ₁ im][C(SO ₂ CF ₃) ₃]	4.4264	3.6960	-13.5083	-9.7043	-50.3203	-48.5232	-2.0089	0.1341
[C ₉ C ₁ im][CH ₃ SO ₄]	6.1957	3.2560	-14.8969	-5.2722	-50.3203	-71.0882	-1.7245	0.1783
[C ₉ C ₁ im][BF ₄]	5.6976	2.0180	-14.4355	-3.4777	-50.3203	-62.9105	-3.0837	0.0458
[C ₉ C ₁ im][C ₃ F ₇ CO ₂]	5.3544	3.1209	-13.8288	-6.2802	-50.3203	-61.9876	-1.9997	0.1354
[C ₉ C ₁ im][CF ₃ SO ₃]	5.3492	2.5464	-14.2281	-5.0089	-50.3203	-60.9237	-2.7825	0.0619
[C ₉ C ₁ im][PO ₂ (C ₂ F ₅) ₂]	4.6883	3.2489	-13.4941	-7.9086	-50.3203	-54.2051	-2.0656	0.1267
[C ₉ C ₁ im][CF ₃ CO ₂]	5.8365	2.5961	-14.3285	-4.2353	-50.3203	-64.7784	-2.2482	0.1056
[C ₉ C ₁ im][SCN]	6.1220	2.2415	-15.7765	-4.6344	-50.3203	-64.8886	-2.4563	0.0858
[C ₉ C ₁ im][CH(CF ₃ SO ₂) ₂]	4.6240	3.3028	-13.8048	-8.1416	-50.3203	-51.9108	-2.2462	0.1058
[C ₉ C ₁ im][C(CN) ₃]	5.4184	2.7581	-14.7936	-6.1745	-50.3203	-53.5982	-2.9991	0.0498
[C ₉ C ₁ im][N(CF ₃ SO ₂) ₂]	4.6707	3.2554	-13.7471	-7.7920	-50.3203	-52.0438	-2.2802	0.1023
[C ₉ C ₁ im][B(C ₂ O ₄) ₂]	5.0565	2.9035	-14.2440	-7.0047	-50.3203	-51.5885	-2.7199	0.0659
[C ₉ C ₁ im][B(CN) ₄]	5.1675	3.1085	-14.7217	-7.9104	-50.3203	-49.0681	-2.6573	0.0701
[C ₉ C ₁ im][NO ₃]	6.4420	2.4056	-14.7697	-3.0774	-50.3203	-69.3606	-1.6274	0.1964
[C ₉ C ₁ im][NO ₂]	7.1498	2.7987	-14.9327	-2.6581	-50.3203	-74.2878	-0.8868	0.4120

Table S5. Experimental and predicted ionic conductivity values from COSMO model, model by Chen *et al.*,²³ model by Gharagheizi *et al.*,³³ and present work for 2 ILs at 0.1 MPa

Ionic Liquids	T/K	$\sigma_{exp}/S \cdot m^{-1}$	$\sigma_{pred,COSMO}/S \cdot m^{-1}$	$\sigma_{pred,Chen,et\,al.}/S \cdot m^{-1}$	$\sigma_{pred,Gharagheizi,et\,al.}/S \cdot m^{-1}$	$\sigma_{pred,present\,work}/S \cdot m^{-1}$
[C ₄ C ₁ im][CH ₃ CO ₂]	288.15	0.0190	0.0756	0.0210	0.0194	0.0212
[C ₄ C ₁ im][CH ₃ CO ₂]	298.15	0.0420	0.1346	0.0490	0.0422	0.0454
[C ₄ C ₁ im][CH ₃ CO ₂]	308.15	0.0830	0.2238	0.0970	0.0830	0.0877
[C ₄ C ₁ im][CH ₃ CO ₂]	318.15	0.1540	0.3511	0.1700	0.1490	0.1549
[C ₄ C ₁ im][CH ₃ CO ₂]	328.15	0.2470	0.5232	0.2710	0.2462	0.2537
[C ₄ C ₁ im][CH ₃ CO ₂]	338.15	0.3720	0.7458	0.3950	0.3777	0.3897
[C ₄ C ₁ im][CH ₃ CO ₂]	348.15	0.5360	1.0226	0.5360	0.5431	0.5674
[C ₄ C ₁ im][CH ₃ CO ₂]	358.15	0.7360	1.3551	0.6820	0.7382	0.7894
[C ₄ C ₁ im][CF ₃ SO ₃]	278.15	0.1038	0.1526	0.1060	0.1043	0.1006
[C ₄ C ₁ im][CF ₃ SO ₃]	288.15	0.1808	0.2675	0.1810	0.1754	0.1863
[C ₄ C ₁ im][CF ₃ SO ₃]	298.15	0.2900	0.4383	0.2880	0.2736	0.3118
[C ₄ C ₁ im][CF ₃ SO ₃]	308.15	0.4360	0.6775	0.4340	0.4019	0.4796
[C ₄ C ₁ im][CF ₃ SO ₃]	318.15	0.6210	0.9959	0.6230	0.5636	0.6881
[C ₄ C ₁ im][CF ₃ SO ₃]	328.15	0.8480	1.4013	0.8580	0.7625	0.9329
[C ₄ C ₁ im][CF ₃ SO ₃]	338.15	1.1170	1.8980	1.1400	1.0035	1.2087
[C ₄ C ₁ im][CF ₃ SO ₃]	348.15	1.4260	2.4866	1.4680	1.2921	1.5103
[C ₄ C ₁ im][CF ₃ SO ₃]	358.15	1.7750	3.1639	1.8390	1.6336	1.8335
[C ₄ C ₁ im][CF ₃ SO ₃]	368.15	2.1600	3.9235	2.2470	2.0316	2.1752

Table S6. 37 support vectors with respective interaction energies, dielectric energy, inverse temperature and coefficient

Support Vector	Interaction Energy/ $kcal \cdot mol^{-1}$						$1/T$	a_i
	$E_{MF,Cation}$	$E_{MF,Anion}$	$E_{vdW,Cation}$	$E_{vdW,Anion}$	$E_{Diel,Cation}$	$E_{Diel,Anion}$		
1	5.2810	1.5133	-9.0277	-3.3559	-50.0718	-62.9105	0.0031	-120.7303
2	5.1545	1.6427	-11.4416	-3.4973	-50.1150	-62.9105	0.0035	1024.0000
3	7.7444	3.7652	-10.0962	-4.1826	-50.0718	-79.6259	0.0035	-406.2031
4	8.0141	3.9206	-9.8350	-4.0761	-50.0718	-79.6259	0.0032	300.9948
5	4.2526	5.1387	-7.7526	-12.4516	-50.6750	-72.5310	0.0034	52.2499
6	5.3886	2.3907	-9.0956	-4.1631	-50.0718	-64.7784	0.0032	522.3277
7	7.0009	3.7645	-7.8316	-4.8269	-50.6750	-76.8542	0.0034	42.4118
8	2.5275	4.6340	-6.3436	-9.5153	-50.6750	-41.7902	0.0036	27.8009
9	3.0450	5.0327	-5.8761	-8.7314	-50.6750	-41.7902	0.0028	-21.7742
10	3.6582	4.3155	-10.1368	-9.4516	-50.1150	-41.7902	0.0034	147.2653
11	3.9656	4.5156	-9.6687	-8.9911	-50.1150	-41.7902	0.0029	-143.8745
12	5.2901	3.3808	-7.7509	-6.3431	-50.6750	-72.0671	0.0034	-66.3771
13	5.5113	3.5427	-7.5446	-6.1677	-50.6750	-72.0671	0.0031	11.8034
14	3.9164	4.3404	-8.0666	-8.9189	-50.0718	-50.3323	0.0029	55.6509
15	3.8423	4.2502	-8.1643	-9.0388	-50.0718	-50.3323	0.0030	87.4035
16	3.3067	3.5908	-8.7222	-9.7425	-50.0718	-50.3323	0.0037	-982.2992
17	4.3108	1.7987	-8.4385	-4.0022	-50.0718	-56.5914	0.0030	75.0997
18	4.3933	1.8652	-8.3373	-3.9527	-50.0718	-56.5914	0.0029	110.8266
19	4.4742	1.9321	-8.2341	-3.9022	-50.0718	-56.5914	0.0028	254.4568
20	4.2679	1.6843	-11.0783	-4.2914	-50.1150	-56.5914	0.0036	-1024.0000
21	4.3737	1.7474	-10.9788	-4.2523	-50.1150	-56.5914	0.0035	-361.8471
22	5.6806	1.6143	-9.6743	-4.6866	-50.1735	-64.8886	0.0034	-25.3793
23	3.0226	3.1181	-6.8226	-7.7581	-50.6750	-52.0438	0.0034	-129.4555
24	3.4177	2.9425	-8.9542	-7.9471	-50.0718	-52.0438	0.0037	1024.0000
25	3.5579	3.0891	-8.8394	-7.8275	-50.0718	-52.0438	0.0035	216.5822
26	3.8926	3.0208	-10.9313	-7.9313	-50.1150	-52.0438	0.0036	293.0616
27	4.9553	4.0325	-9.5051	-6.7917	-50.1150	-52.0438	0.0025	56.9571
28	3.4065	2.5715	-7.9250	-8.4625	-50.6750	-49.0681	0.0036	87.8615
29	3.9899	3.1308	-7.2846	-7.8305	-50.6750	-49.0681	0.0028	40.7075

30	6.1801	2.1679	-12.6341	-3.2767	-50.2776	-62.9105	0.0029	-105.7965
31	5.8173	2.0159	-13.1014	-3.3981	-50.2776	-62.9105	0.0031	-34.3757
32	5.9414	2.0666	-12.9497	-3.3587	-50.2776	-62.9105	0.0030	-54.2756
33	4.2538	2.0489	-9.3551	-5.1213	-50.0718	-60.9237	0.0037	19.9874
34	4.7311	2.3647	-8.9720	-4.9013	-50.0718	-60.9237	0.0032	-77.3488
35	4.9314	2.5029	-8.7743	-4.7877	-50.0718	-60.9237	0.0030	-1024.0000
36	5.1946	2.1864	-12.6032	-4.1164	-50.2776	-56.5914	0.0031	221.4790
37	4.5450	3.2868	-12.6672	-7.7409	-50.2776	-52.0438	0.0033	-95.1906
