

Supporting Information for: “Appraisal of dispersion damping functions for the effective fragment potential method”

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The IL195×8 data set is assembled here for the first time. Its structures (195 distinct ion pairs) represent a subset of the IL-2013 database¹, which we have then shifted along the vector between the cation and anion centers of mass to generate ions pairs at different intermolecular separations: $0.90R_e$, $0.95R_e$, R_e , $1.05R_e$, $1.10R_e$, $1.25R_e$, $1.50R_e$, and $2.00R_e$, where R_e is the equilibrium center-of-mass separation. Benchmark interaction energies were computed using coupled-cluster theory with single, double, and perturbative triple excitations [CCSD(T)], within the domain-localized pair natural orbital (DLPNO) approximation.^{2,3} We employ tight PNO cutoffs (**TightSCF** and **TightPNO** in the ORCA software⁴), as non-bonded interaction energies are known to be very sensitive to this threshold.^{5,6} We use the noniterative triples correction (sometimes called T_0). Previous work on ionic liquid benchmarks has demonstrated that when tight DLPNO thresholds are used, the locality error incurred with respect to canonical CCSD(T) results is on the order of ~ 0.1 kJ/mol, in systems whose interaction energies are tens of kcal/mol.⁷ We did not employ the chain-of-spheres exchange approximation in the HF calculations.⁸

To obtain CCSD(T) energies in the complete basis set (CBS) limit, we use a CCSD(T) correction to the CBS-extrapolated MP2 result:

$$E_{\text{int}}^{\text{CCSD(T)/CBS}} = E_{\text{int}}^{\text{MP2/CBS}} + \delta E_{\text{CCSD(T)}} \quad (\text{S1})$$

where

$$\delta E_{\text{CCSD(T)}} = E_{\text{corr}}^{\text{CCSD(T)/aTZ}} - E_{\text{corr}}^{\text{MP2/aTZ}}. \quad (\text{S2})$$

Here, “aTZ” indicates that the aug-cc-pVTZ basis set⁹ is used to evaluate $\delta E_{\text{CCSD(T)}}$. To obtain $E_{\text{int}}^{\text{MP2/CBS}}$, the Hartree-Fock (HF) energy is first extrapolated to the CBS limit using a two-point scheme involving the aug-cc-pVTZ and aug-cc-pVQZ basis sets:¹⁰

$$E^{\text{HF/CBS}} = \frac{E^{\text{HF/aTZ}} e^{-\alpha\sqrt{Y}} - E^{\text{HF/aQZ}} e^{-\alpha\sqrt{X}}}{e^{-\alpha\sqrt{Y}} - e^{-\alpha\sqrt{X}}}. \quad (\text{S3})$$

The MP2 correlation energy is evaluated within the resolution-of-identity (RI) approximation, using the same two basis sets but via the extrapolation formula:¹⁰

$$E_{\text{corr}}^{\text{MP2/CBS}} = \frac{X^\beta E_{\text{corr}}^{\text{MP2/aTZ}} - Y^\beta E_{\text{corr}}^{\text{MP2/aQZ}}}{X^\beta - Y^\beta}. \quad (\text{S4})$$

In these formulas, $X = 3$ for aug-cc-pVTZ, $Y = 4$ for aug-cc-pVQZ, and the parameters $\alpha = 5.79$ and $\beta = 3.05$ are taken from Ref. 10.

The benchmarks interaction energies are provided in Table S1. These represent DLPNO(**TightPNO**) CCSD(T)/CBS estimates, as described above, except in the case of the $R = 2.00R_e$ data points for IL96, IL102, and IL103. In those cases, unrealistically large correlation energies are obtained from the DLPNO-CCSD(T)/aug-cc-pVTZ calculations, which causes $\delta E_{\text{CCSD(T)}}$ to be artificially large. As a consequence, these data points were treated at the RI-MP2/CBS level.

Table S1: DLPNO(TightPNO) CCSD(T)/CBS benchmark interaction energies (in kcal/mol) for the IL195×8 data set

Structure	Intermolecular Separation / R_e							
	0.90	0.95	1.00	1.05	1.10	1.25	1.50	2.00
IL1	-84.6254	-89.3084	-90.4062	-89.4366	-87.3115	-79.0847	-66.6431	-50.5833
IL2	-85.2374	-89.4101	-90.3889	-89.5017	-87.5757	-79.7300	-67.3886	-51.0942
IL3	-82.3008	-87.7206	-88.9523	-87.8185	-85.5686	-76.9187	-64.2966	-48.4034
IL4	-85.6194	-89.3861	-90.2873	-89.4788	-87.7060	-80.2764	-68.2622	-52.0782
IL5	-84.0309	-88.7478	-89.8659	-88.8747	-86.7921	-78.5694	-66.1346	-50.1782
IL6	-86.1043	-89.3848	-90.1911	-89.4748	-87.8882	-81.0980	-69.6255	-53.4627
IL7	-83.5940	-88.4585	-89.5725	-88.6030	-86.5237	-78.2901	-65.8739	-49.8551
IL8	-81.8487	-85.9717	-87.0890	-86.4464	-84.7616	-77.5165	-66.1517	-51.1278
IL9	-75.4897	-82.9886	-84.4482	-83.0031	-80.1832	-70.3204	-57.6854	-43.0885
IL10	-82.5170	-85.6291	-86.5838	-86.1225	-84.8777	-78.9728	-68.7297	-53.7043
IL11	-82.1403	-85.3054	-86.2032	-85.7195	-84.3200	-78.0921	-67.5501	-52.3758
IL12	-82.9056	-86.1413	-87.1192	-86.6138	-85.2261	-78.7976	-67.9117	-52.7481
IL13	-81.4394	-85.2689	-86.3520	-85.8241	-84.2983	-77.3661	-66.0855	-50.8436
IL14	-80.3153	-84.7018	-85.8858	-85.2561	-83.4993	-76.0074	-64.4629	-49.5499
IL15	-79.1083	-83.9159	-85.2455	-84.6033	-82.8318	-75.2960	-63.7909	-48.8719
IL16	-82.2216	-85.1482	-86.0973	-85.7215	-84.5345	-79.0207	-69.1255	-54.2296
IL17	-82.3019	-84.8992	-85.7162	-85.3601	-84.2137	-78.7903	-69.0896	-54.5532
IL18	-78.2289	-83.7660	-85.0649	-84.0133	-81.7438	-73.0924	-60.9176	-46.1568
IL19	-84.0890	-86.7901	-87.6956	-87.3663	-86.2954	-80.7434	-70.4099	-55.0184
IL20	-79.9290	-84.2708	-85.4559	-84.8759	-83.2206	-76.0045	-64.6454	-49.6366
IL21	-77.5256	-83.0246	-84.5507	-83.8518	-81.9351	-73.9691	-62.1685	-47.0892
IL22	-82.5844	-85.1279	-85.9758	-85.6921	-84.6714	-79.6787	-70.4678	-55.7163
IL23	-84.5578	-86.8872	-87.7092	-87.4818	-86.6095	-81.7979	-72.2687	-57.0582
IL24	-78.6477	-83.7856	-85.2468	-84.5497	-82.7056	-74.9556	-63.1157	-47.7872
IL25	-91.6571	-97.5407	-99.0457	-98.0425	-95.6917	-85.9678	-71.4299	-53.1339
IL26	-92.3492	-97.6187	-98.9874	-98.0488	-95.8942	-86.6414	-72.1902	-53.5965
IL27	-89.3961	-95.8733	-97.5414	-96.5058	-94.0542	-84.0757	-69.4811	-51.5301
IL28	-93.2643	-98.0160	-99.3371	-98.5207	-96.4948	-87.6576	-73.4079	-54.7688
IL29	-88.4172	-95.1603	-96.9137	-95.8570	-93.3668	-83.2757	-68.6580	-50.8148
IL30	-93.8753	-98.0651	-99.2214	-98.5209	-96.7300	-88.6147	-74.9426	-56.3374
IL31	-86.7057	-94.5328	-96.5002	-95.3741	-92.6706	-82.0158	-66.9960	-49.0405
IL32	-73.4711	-80.9844	-83.4545	-83.0500	-81.1043	-72.6519	-60.3130	-45.4009
IL33	-62.6665	-77.4331	-80.9041	-79.5272	-76.1364	-64.7799	-51.6178	-37.5946
IL34	-69.5571	-79.2617	-81.8112	-80.5601	-77.6051	-67.0900	-53.9967	-39.5861
IL35	-74.5481	-81.3632	-83.6481	-83.3370	-81.6345	-73.7527	-61.6019	-46.3095
IL36	-66.5566	-78.3751	-81.5271	-80.4092	-77.4686	-66.6797	-53.3641	-39.0282
IL37	-69.6937	-79.3063	-81.7983	-80.6728	-77.7758	-67.1931	-53.8473	-39.3506
IL38	-67.5516	-78.5062	-81.7111	-80.9831	-78.4098	-68.6492	-55.9803	-41.5771
IL39	-75.2428	-81.5598	-83.7758	-83.5525	-81.9483	-74.4464	-62.4309	-46.9982
IL40	-68.8269	-78.9510	-81.7960	-80.8516	-78.1784	-67.7749	-54.4301	-39.9406
IL41	-69.6517	-79.3540	-81.8067	-80.8171	-78.0405	-67.6429	-54.3395	-39.7501
IL42	-64.5865	-76.7181	-80.1385	-79.3659	-76.6728	-66.7798	-54.3041	-40.2191
IL43	-76.5856	-83.3129	-84.9190	-83.8412	-81.4965	-72.6858	-60.3851	-45.3247
IL44	-77.4910	-83.4593	-84.9728	-84.0287	-81.8847	-73.5078	-61.2604	-45.9916
IL45	-74.1880	-81.6669	-83.4372	-82.2950	-79.8391	-70.8361	-58.6073	-43.8207
IL46	-75.0237	-80.4376	-81.7648	-80.8919	-78.9055	-71.1686	-59.7570	-45.2914
IL47	-72.8180	-80.9049	-82.8150	-81.6385	-79.1297	-70.0174	-57.7490	-42.9712
IL48	-79.0806	-83.7914	-85.0349	-84.3458	-82.5693	-75.1407	-63.5069	-48.2372
IL49	-70.8673	-80.3338	-82.4805	-81.2179	-78.5240	-69.0114	-56.4576	-41.5395
IL50	-79.3453	-93.6190	-97.0577	-95.4123	-91.5732	-77.9733	-60.8957	-42.5054
IL51	-83.1145	-88.1487	-88.5369	-86.5049	-83.3996	-73.0515	-59.6481	-44.0805
IL52	-79.7679	-85.9561	-86.6249	-84.5225	-81.2173	-70.3225	-56.7474	-41.4092
IL53	-82.8957	-87.5407	-87.8021	-85.7590	-82.6876	-72.4807	-59.2918	-43.9621
IL54	-77.1545	-83.6529	-84.4076	-82.3784	-79.2076	-68.9477	-56.1841	-41.5462
IL55	-79.0202	-85.1571	-85.8100	-85.7380	-80.4692	-69.7577	-56.4439	-41.3961
IL56	-83.3509	-87.3773	-87.4954	-85.5237	-82.5532	-72.6040	-59.5736	-44.2988
IL57	-77.6711	-83.3194	-83.8739	-81.8548	-78.7380	-68.6319	-56.0099	-41.5236

IL58	-79.1736	-84.8743	-85.4467	-83.4377	-80.2700	-69.8350	-56.7086	-44.2545
IL59	-83.2831	-87.1052	-87.1983	-85.2548	-82.3400	-72.4924	-59.4878	-44.1961
IL60	-78.5076	-83.1832	-83.5657	-81.6490	-78.6897	-68.9484	-56.5282	-42.0994
IL61	-78.9593	-84.5831	-85.1546	-83.1892	-80.0776	-69.7302	-56.6578	-59.2153
IL62	-79.2156	-83.3622	-83.4986	-81.5679	-78.6854	-69.0381	-56.5310	-41.9326
IL63	-82.6575	-85.2823	-84.9877	-83.1161	-80.4744	-71.4871	-59.1137	-43.9669
IL64	-75.6959	-79.8860	-79.9593	-77.9356	-74.9519	-65.3000	-53.1991	-39.4326
IL65	-82.3312	-85.0348	-84.8146	-82.9448	-80.2824	-71.1992	-58.6747	-43.4437
IL66	-77.8173	-82.1670	-82.3249	-80.3507	-77.4420	-67.8157	-55.4101	-40.9889
IL67	-81.2497	-83.4630	-83.0617	-81.2215	-78.6294	-69.8132	-57.6928	-43.0546
IL68	-77.8048	-82.1631	-82.3225	-80.3490	-77.4434	-67.8186	-55.4111	-40.9860
IL69	-81.2591	-83.4661	-83.0570	-81.2142	-78.6229	-69.8050	-57.6849	-43.0486
IL70	-81.3026	-84.1605	-83.8982	-81.9833	-79.2947	-70.2346	-57.8885	-42.9647
IL71	-81.2938	-84.1609	-83.9027	-81.9876	-79.2980	-70.2389	-57.8898	-42.9649
IL72	-79.5722	-82.6485	-82.4984	-80.5805	-77.8408	-68.6557	-56.4481	-41.9590
IL73	-80.4704	-82.8877	-82.4937	-80.5768	-77.8882	-68.8184	-56.5797	-41.9676
IL74	-80.1269	-83.1251	-82.9479	-81.0330	-78.2903	-69.1085	-56.8387	-42.2601
IL75	-73.0794	-76.9356	-76.8757	-74.8292	-71.8858	-62.6002	-51.1163	-38.1000
IL76	-79.1809	-82.2593	-82.0603	-80.1647	-77.4568	-68.4733	-56.3874	-41.8694
IL77	-80.9221	-83.8905	-83.6032	-81.6150	-78.8595	-69.6270	-57.1472	-42.2014
IL78	-80.1293	-81.8081	-81.3834	-79.7505	-77.4844	-69.7318	-58.4669	-44.0097
IL79	-80.0612	-82.5347	-82.1361	-80.1997	-77.4838	-68.3851	-56.1128	-41.4788
IL80	-80.0545	-82.7891	-82.5159	-80.5910	-77.8902	-68.7886	-56.5508	-41.9455
IL81	-80.0581	-82.5360	-82.1388	-80.2039	-77.4828	-68.3878	-56.1145	-41.4838
IL82	-80.6262	-82.9050	-82.6125	-80.8250	-78.3425	-69.8103	-57.9166	-43.2913
IL83	-80.2545	-83.4566	-83.1702	-81.1060	-78.2608	-68.8034	-56.1497	-41.1394
IL84	-89.6082	-95.9137	-96.4944	-94.1707	-90.5656	-78.4690	-63.0002	-45.5992
IL85	-81.2527	-91.7977	-93.4062	-90.9947	-86.9687	-74.0433	-58.7114	-42.0460
IL86	-90.0157	-95.6055	-95.9762	-93.6764	-90.1441	-78.2181	-62.9323	-45.6735
IL87	-84.8968	-91.6693	-92.3044	-89.9310	-86.2678	-74.4409	-59.7158	-43.2564
IL88	-83.0579	-91.8681	-93.0215	-90.6677	-86.8000	-74.2535	-59.1016	-42.5004
IL89	-90.9672	-95.6289	-95.7827	-93.5468	-90.1368	-78.5660	-63.4245	-46.1389
IL90	-85.0028	-91.1537	-91.7127	-89.3657	-85.7647	-74.0730	-59.4853	-43.2001
IL91	-83.5518	-91.7671	-92.8067	-90.5114	-86.7577	-74.4687	-59.4763	-42.9256
IL92	-90.9656	-95.3133	-95.3777	-93.1720	-89.8045	-78.3136	-63.1779	-45.8822
IL93	-85.9323	-91.0979	-91.4407	-89.1990	-85.7856	-74.4584	-60.0389	-43.7640
IL94	-83.6707	-91.5030	-92.4872	-90.2260	-86.5424	-74.3899	-59.4577	-42.9490
IL95	-73.7020	-79.3285	-79.4917	-77.1292	-73.7625	-63.3936	-51.0781	-37.6568
IL96	-71.5016	-77.8115	-78.2009	-75.8254	-72.3467	-61.8287	-49.4327	-36.0019 ^a
IL97	-70.5132	-78.2379	-78.9882	-76.7143	-73.2399	-62.5562	-50.1175	-36.5848
IL98	-72.0987	-78.3958	-78.7365	-76.2466	-72.6120	-61.6279	-49.0046	-35.8546
IL99	-73.8764	-79.3400	-79.1895	-76.5798	-73.0000	-62.5013	-50.3536	-36.9992
IL100	-70.8033	-77.1911	-77.4487	-74.9873	-71.5222	-61.0200	-48.9246	-37.6819
IL101	-71.3265	-77.1487	-77.3997	-75.0398	-71.6748	-61.4346	-49.5532	-36.4141
IL102	-70.6011	-76.3314	-76.5428	-74.0514	-70.5484	-60.0230	-48.0623	-35.1600 ^a
IL103	-68.3465	-76.5455	-77.0720	-74.3961	-70.5684	-59.5369	-47.2843	-34.2735 ^a
IL104	-74.0642	-79.1596	-79.0836	-76.4252	-73.0283	-62.6647	-50.5625	-37.2431
IL105	-75.8270	-82.1367	-82.6027	-80.3344	-76.9626	-66.4587	-53.7727	-39.7844
IL106	-72.7591	-80.1709	-80.9811	-78.7239	-75.1881	-64.3012	-51.5079	-37.4362
IL107	-73.5562	-80.6109	-81.3431	-79.1311	-75.7638	-65.3783	-53.0090	-39.0735
IL108	-70.1746	-77.8810	-78.7096	-76.4515	-73.0991	-62.8478	-50.8306	-37.3901
IL109	-72.1732	-79.3613	-80.1108	-77.8695	-74.3910	-63.7059	-51.1836	-37.3727
IL110	-76.1776	-81.4726	-81.7377	-79.5513	-76.3199	-66.1712	-53.7958	-39.7584
IL111	-70.4911	-77.4757	-78.1457	-75.8922	-72.5895	-62.4902	-50.6481	-37.3714
IL112	-72.4640	-79.1693	-79.8232	-77.6312	-74.2474	-63.7857	-51.4092	-37.6684
IL113	-76.1300	-81.1818	-81.4220	-79.2778	-76.0784	-65.9976	-53.6489	-39.6242

IL114	-71.4489	-77.4264	-77.9314	-75.7822	-72.6383	-62.8240	-51.1284	-38.4441
IL115	-72.5387	-79.0045	-79.6109	-77.4469	-74.1043	-63.7251	-51.4082	-37.6812
IL116	-73.3950	-91.8627	-94.2371	-90.4219	-84.7650	-68.8523	-52.3521	-35.9179
IL117	-77.2286	-91.9355	-93.5617	-89.8720	-84.4344	-68.9701	-52.6614	-36.2939
IL118	-69.8078	-87.3345	-89.4640	-85.7173	-80.2567	-65.2723	-49.8619	-34.4116
IL119	-96.1267	-113.1117	-113.5531	-108.0633	-100.8660	-81.2162	-61.0093	-41.6714
IL120	-106.2820	-117.3546	-117.2611	-112.3210	-105.6669	-86.3634	-65.2998	-44.7820
IL121	-114.1052	-121.4438	-120.3861	-115.6039	-109.4217	-91.1298	-70.0322	-48.4359
IL122	-90.5647	-108.7725	-109.3623	-103.7832	-96.5769	-77.3450	-58.0618	-40.6155
IL123	-100.9272	-112.8334	-112.7554	-107.6368	-100.8721	-81.7761	-61.6219	-46.6655
IL124	-108.4106	-117.2092	-116.4691	-111.6157	-105.2738	-86.8454	-66.2282	-45.6014
IL125	-77.7760	-100.0008	-103.8924	-100.5924	-94.7473	-77.1425	-58.5371	-40.6884
IL126	-90.8687	-94.0341	-94.4951	-93.3475	-91.3476	-83.3803	-71.1653	-54.8582
IL127	-74.6972	-84.8894	-86.8774	-84.9974	-81.4850	-69.7902	-55.5205	-40.1283
IL128	-78.2131	-84.4382	-86.2582	-85.5692	-83.5922	-75.3356	-63.1505	-47.7110
IL129	-83.6255	-101.8787	-104.9059	-101.7809	-96.4990	-80.1397	-61.9547	-43.3876
IL130	-72.8725	-84.5499	-87.0005	-85.4085	-82.1069	-70.7638	-56.5253	-40.6085
IL131	-89.4693	-94.7786	-95.9186	-94.6434	-92.0721	-81.9613	-67.1242	-48.9421
IL132	-82.8712	-89.5757	-90.6549	-88.8813	-85.7604	-75.0047	-60.9896	-44.9492
IL133	-71.7953	-98.2827	-102.8031	-99.1797	-92.9630	-74.9186	-56.4346	-38.9494
IL134	-92.2950	-95.7622	-96.1926	-94.8177	-92.4545	-83.5660	-70.4837	-53.6678
IL135	-61.1102	-88.2481	-93.0159	-89.7037	-84.2217	-68.3629	-52.4120	-36.7596
IL136	-83.3985	-89.1737	-90.1693	-88.6365	-85.8447	-75.9849	-62.5012	-46.3294
IL137	-61.3113	-94.5737	-100.6590	-96.9026	-90.2076	-71.5507	-53.4196	-36.5491
IL138	-59.2654	-86.1862	-91.2517	-88.1318	-82.5105	-66.6329	-50.8606	-35.6240
IL139	-96.1461	-102.4883	-103.4386	-101.5119	-98.1946	-86.5499	-70.6011	-51.4015
IL140	-78.3528	-90.5894	-92.9262	-90.8915	-87.1124	-74.5374	-59.2046	-42.3544
IL141	-63.2898	-94.6847	-100.0137	-95.8816	-88.9558	-69.8977	-51.8369	-35.4582
IL142	-87.9044	-99.3231	-101.7713	-99.8252	-95.9557	-82.4276	-65.2452	-46.5932
IL143	-74.2204	-90.8107	-93.7287	-91.0828	-86.4952	-72.4574	-56.7471	-40.2089
IL144	-80.7816	-86.2814	-87.5796	-86.4485	-84.0226	-74.5064	-60.9130	-44.8217
IL145	-51.2325	-84.6925	-90.8077	-87.2554	-81.0214	-64.2232	-48.3880	-33.4542
IL146	-95.3833	-104.1561	-105.7754	-103.7850	-100.0735	-87.0107	-69.8364	-50.1429
IL147	-79.4737	-91.0983	-93.3032	-91.1551	-87.2176	-74.5048	-59.1259	-42.2182
IL148	-55.1525	-93.3706	-99.7241	-95.2107	-87.7907	-68.1236	-50.1606	-34.0701
IL149	-61.0864	-96.2615	-102.0947	-97.9829	-91.0935	-72.0232	-53.5208	-36.4702
IL150	-81.8541	-92.5168	-94.6205	-92.6368	-88.9248	-76.5494	-61.2496	-44.1434
IL151	-82.7972	-92.3934	-94.3719	-92.6184	-89.1494	-77.1903	-62.0114	-44.8298
IL152	-46.2645	-92.0965	-99.9759	-95.5825	-88.0167	-68.2738	-50.2212	-33.9089
IL153	-43.0817	-83.4740	-90.4902	-86.5633	-79.9030	-62.6973	-46.9586	-32.2762
IL154	-92.6824	-103.2629	-105.2522	-102.9587	-98.8376	-84.9568	-67.4811	-47.9488
IL155	-73.2192	-90.2775	-93.3321	-90.6000	-85.9381	-71.7573	-56.0396	-39.4812
IL156	-97.1360	-106.9803	-108.9550	-106.8165	-102.8562	-88.4835	-69.9408	-49.9749
IL157	-90.0421	-98.8290	-100.8177	-99.2002	-95.6892	-82.8996	-66.2395	-47.9382
IL158	-98.0401	-108.6044	-110.9476	-109.0108	-105.0260	-90.5899	-71.7984	-51.2922
IL159	-78.5166	-95.4404	-99.0509	-96.7839	-92.1558	-77.1534	-60.0987	-42.5351
IL160	-95.9954	-105.7596	-107.6458	-105.5002	-101.4352	-86.9708	-68.4657	-48.8203
IL161	-87.0116	-96.9038	-99.1925	-97.6300	-94.2218	-81.7011	-65.3894	-47.5065
IL162	-96.4548	-107.4804	-109.9232	-108.0089	-103.9935	-89.5630	-70.8632	-50.5255
IL163	-75.9941	-93.8492	-97.5965	-95.2994	-90.7215	-75.9183	-59.1119	-41.7984
IL164	-88.8590	-92.1666	-92.6112	-91.2086	-88.7902	-79.4074	-65.3178	-48.1917
IL165	-81.6745	-86.7126	-87.7190	-86.4584	-84.0248	-74.7962	-61.6371	-45.9493
IL166	-91.8621	-96.6405	-97.5082	-96.1189	-93.4915	-83.3151	-68.3018	-50.1521
IL167	-79.0762	-85.4011	-86.6852	-85.4123	-82.7769	-72.8262	-59.0971	-43.2454
IL168	-94.2267	-106.9735	-109.5834	-107.1174	-102.4192	-86.1858	-66.6965	-46.8326

IL169	-83.5904	-97.0717	-99.9788	-97.9241	-93.6799	-79.3506	-62.3616	-44.5965
IL170	-93.5821	-107.9246	-110.8826	-108.3891	-103.5246	-87.0113	-67.3687	-47.1021
IL171	-68.9418	-92.9806	-97.7634	-94.9415	-89.5944	-73.4850	-56.4594	-39.8602
IL172	-84.7708	-89.1989	-89.9717	-88.5665	-85.9573	-75.8764	-61.2934	-44.3846
IL173	-78.6745	-84.3214	-85.6102	-84.4139	-81.8686	-72.3266	-59.2683	-43.9992
IL174	-87.5855	-93.1511	-94.2192	-92.7142	-89.8763	-79.1727	-64.3832	-47.0390
IL175	-72.6664	-81.6748	-83.4936	-81.8005	-78.5884	-67.5544	-53.7706	-38.6066
IL176	-96.1354	-109.5734	-112.1121	-109.3943	-104.4212	-87.5698	-67.4204	-46.9611
IL177	-93.5280	-101.9553	-103.6131	-101.7103	-98.0097	-84.9875	-68.0062	-49.1539
IL178	-98.3458	-111.7869	-114.2296	-111.4909	-106.5366	-89.9794	-69.8761	-48.6662
IL179	-86.9290	-100.4802	-103.4932	-101.3250	-96.8793	-81.6260	-63.4773	-44.6529
IL180	-101.6299	-109.9845	-111.6575	-109.5674	-105.4646	-90.4697	-70.7663	-49.8859
IL181	-93.9007	-101.5482	-103.0895	-101.2925	-97.8024	-85.0432	-68.0935	-49.2783
IL182	-100.1356	-109.8581	-112.0205	-109.8995	-105.6504	-90.0686	-70.0518	-49.0655
IL183	-88.4172	-100.7092	-103.3487	-101.1733	-96.8787	-82.1008	-64.2698	-45.6268
IL184	-96.7924	-107.6193	-109.7440	-107.3066	-102.7230	-86.7656	-67.1198	-47.0167
IL185	-80.6057	-85.3470	-86.6051	-85.8455	-83.7626	-75.3031	-62.4979	-46.8841
IL186	-94.3833	-108.2718	-111.0049	-108.3535	-103.3254	-86.4498	-66.4512	-46.0808
IL187	-79.7057	-96.2485	-99.8644	-97.5447	-92.9533	-77.7545	-60.3846	-42.5515
IL188	-104.0393	-111.8497	-111.5058	-107.4361	-101.8783	-85.1045	-65.6678	-45.7064
IL189	-99.5419	-105.5363	-105.9648	-103.3592	-99.2628	-85.4416	-67.8822	-48.7237
IL190	-100.0474	-108.8153	-110.5444	-108.1409	-103.5977	-87.3976	-67.2018	-46.6424
IL191	-81.0303	-98.2100	-101.8023	-99.2664	-94.3494	-78.4796	-60.3739	-41.7334
IL192	-104.6837	-111.5522	-112.9114	-110.9902	-107.1780	-92.7394	-72.8920	-51.2557
IL193	-96.9074	-103.8365	-105.2952	-103.7084	-100.4332	-87.9051	-70.6287	-51.0188
IL194	-104.3686	-112.7045	-114.3897	-112.1530	-107.9090	-92.1894	-71.5271	-49.5501
IL195	-88.6831	-100.6578	-103.5646	-101.5189	-97.1094	-81.4594	-62.5315	-43.2167

^aData point reported at the RI-MP2/CBS level instead of CCSD(T)/CBS.

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