Assessment of Kohn–Sham Density Functional Theory and Møller–Plesset Perturbation Theory for Ionic Liquids

Supporting Information

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Table 1 shows all cation anion combinations included in the IL–2013 set. All ion pair structures of the benchmark set are included in the *IL-2013-set.xyz* file which can be viewed for example with Molden. Additionally, this file include all reference interaction energies. Table 2 lists all calculated values used to calculate the benchmark interaction energies. Further tables of the supporting information show errors of all validated approaches for each ion pair.

Table 1: Anion-cation-combinations of the IL–2013 benchmark set are listed with a +. Cations and anions are shown in Fig. 1

	C1	**C2**	**C3**	**C4**	**C5**	**C6**	**C7**	**C8**
A1	+	+	+	+	+	+	+	+
A2	+	—	+	—	+	+	+	+
A3	+	—	+	—	+	+	+	+
A4	—	—	+	—	—	—	+	+
A5	+	+	+	+	+	+	+	+
A6	—	+	—	+	—	—	—	—
A7	—	+	—	+	—	—	—	—
A8	—	—	+	—	—	—	+	+
A9	+	—	+	—	+	+	+	+
A10	—	+	—	+	—	—	—	—
A11	—	+	—	+	—	—	—	—
A12	—	+	—	+	—	—	—	—

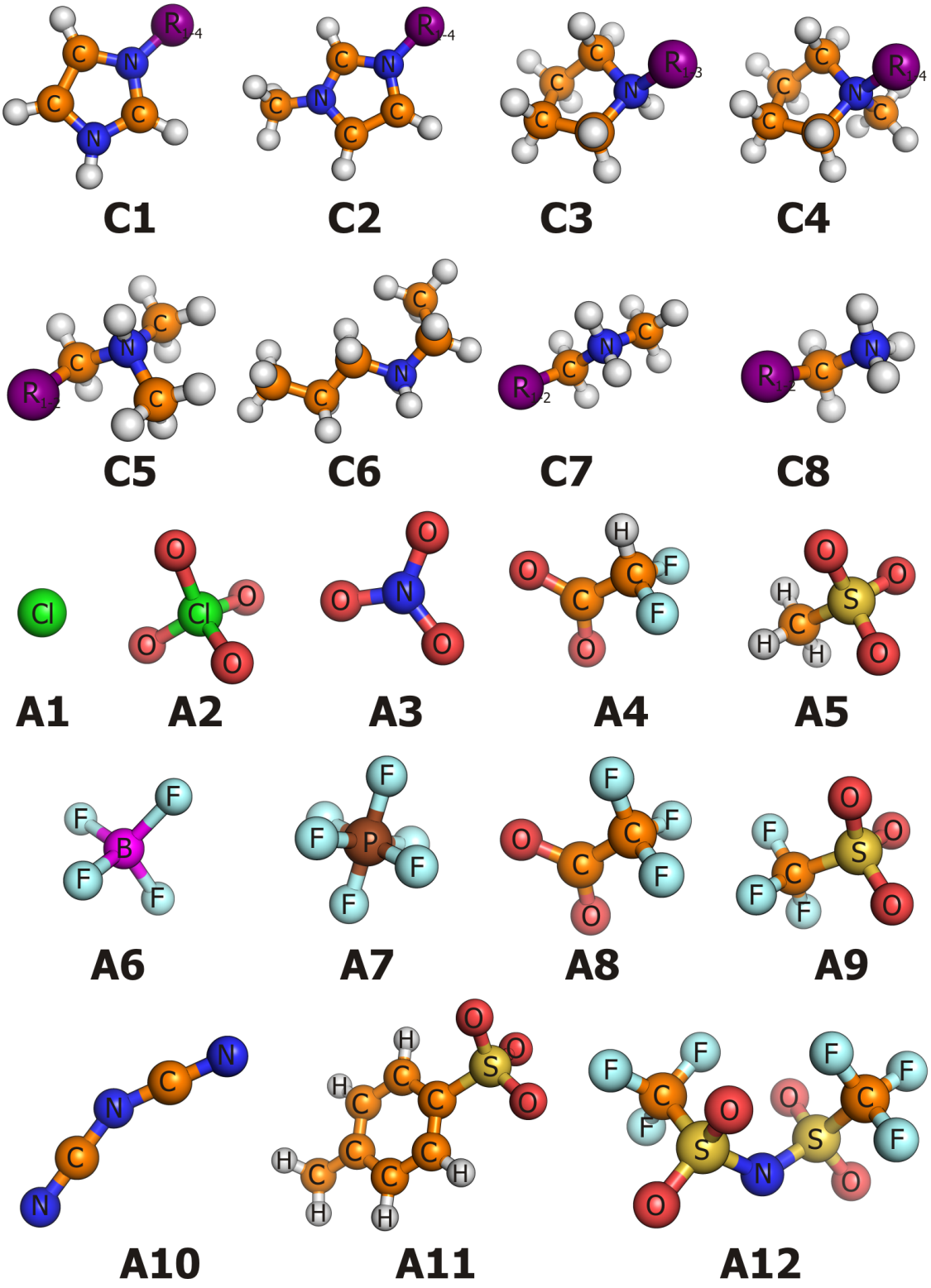

Figure 1: Cations and anions included in the IL–2013 set

Table 2: Interaction energies E in kJ/mol used to calculate the reference energy $E_{CBS}^{CCSD(T)}$ for all structures N of the IL–2013 set. n_{atom} is the number of atoms of the reference structure. All values are counter poise corrected.

N	n_{atom}	$E_{cc-pVTZ}^{MP2}$	$E_{cc-pVQZ}^{MP2}$	E_{CBS}^{MP2}	E_{small}^{MP2}	$E_{small}^{CCSD(T)}$	$E_{CBS}^{CCSD(T)}$
1	21	−370.6	−374.3	−377.1	−359.7	−362.0	−379.3
2	24	−370.3	−373.8	−376.4	−358.6	−360.8	−378.7
3	24	−364.9	−368.1	−370.4	−354.4	−356.7	−372.7
4	27	−369.7	−373.4	−376.0	−357.7	−360.2	−378.5
5	27	−368.5	−371.9	−374.3	−357.3	−359.6	−376.6
6	30	−369.1	−372.8	−375.6	−357.4	−359.7	−378.0
7	30	−367.3	−370.7	−373.2	−356.6	−358.8	−375.4
8	17	−413.0	−416.6	−419.3	−404.7	−405.2	−419.8
9	20	−403.9	−407.6	−410.3	−395.8	−396.2	−410.8
10	20	−411.2	−410.2	−409.4	−395.2	−396.1	−410.3
11	20	−405.8	−405.4	−405.1	−390.9	−391.8	−406.0
12	20	−407.9	−411.4	−413.9	−399.7	−400.1	−414.3
13	23	−402.0	−405.7	−408.4	−387.0	−388.8	−410.2
14	23	−409.1	−408.0	−407.3	−403.6	−404.4	−408.1
15	23	−405.5	−405.7	−405.9	−396.8	−397.6	−406.7
16	23	−408.4	−412.0	−414.5	−393.6	−395.4	−416.4
17	26	−401.4	−405.2	−408.0	−386.5	−388.2	−409.6
18	26	−408.3	−407.7	−407.2	−402.9	−403.8	−408.0
19	26	−405.0	−405.4	−405.6	−395.7	−396.3	−406.2
20	26	−407.2	−410.7	−413.2	−392.3	−394.1	−415.0
21	21	−367.6	−371.9	−375.0	−353.9	−347.7	−368.7
22	21	−355.8	−357.0	−357.9	−349.0	−345.3	−354.1
23	24	−366.3	−370.0	−372.7	−353.4	−346.6	−365.9
24	24	−363.9	−367.5	−370.1	−350.8	−344.7	−364.0
25	24	−368.7	−372.4	−375.1	−355.2	−348.2	−368.2
26	24	−365.2	−368.8	−371.5	−352.4	−345.7	−364.8
27	24	−363.0	−366.9	−369.8	−349.7	−343.4	−363.4
28	24	−360.2	−364.4	−367.4	−346.8	−340.4	−361.0
29	27	−364.3	−367.9	−370.6	−351.3	−344.4	−363.6
30	27	−362.3	−366.3	−369.3	−348.2	−341.2	−362.2

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Table 2 – continued from previous page

N	n_{atom}	$E^{MP2}_{cc-pVTZ}$	$E^{MP2}_{cc-pVQZ}$	E^{MP2}_{CBS}	E^{MP2}_{small}	$E^{CCSD(T)}_{small}$	$E^{CCSD(T)}_{CBS}$
31	27	−359.1	−361.1	−362.6	−349.9	−344.5	−357.2
32	27	−370.8	−374.9	−377.8	−356.4	−349.1	−370.5
33	27	−361.4	−365.3	−368.2	−348.0	−341.3	−361.5
34	27	−357.3	−361.5	−364.5	−344.0	−337.6	−358.1
35	30	−363.9	−367.5	−370.2	−346.5	−340.4	−364.0
36	30	−370.5	−374.9	−378.2	−352.0	−345.6	−371.8
37	30	−360.2	−364.1	−367.0	−343.4	−337.8	−361.4
38	24	−410.6	−414.8	−417.7	−396.5	−396.1	−417.4
39	27	−410.8	−415.0	−418.0	−395.3	−394.4	−417.0
40	27	−404.1	−408.3	−411.3	−390.8	−390.6	−411.1
41	30	−412.1	−416.4	−419.5	−397.3	−396.6	−418.8
42	30	−401.5	−405.6	−408.6	−391.0	−391.0	−408.7
43	33	−411.4	−415.9	−419.1	−396.6	−395.9	−418.4
44	33	−400.1	−403.8	−406.6	−389.4	−389.5	−406.7
45	31	−350.2	−353.1	−355.2	−339.9	−335.8	−351.1
46	31	−339.2	−338.7	−338.3	−340.0	−338.8	−337.1
47	31	−338.1	−340.3	−341.8	−330.1	−330.9	−342.6
48	34	−350.5	−353.6	−355.9	−338.8	−334.7	−351.9
49	34	−341.2	−341.2	−341.2	−338.6	−336.8	−339.5
50	34	−337.9	−340.2	−341.8	−329.6	−330.3	−342.5
51	34	−341.9	−344.9	−347.0	−332.8	−329.7	−343.9
52	37	−351.0	−354.2	−356.6	−338.4	−334.1	−352.3
53	37	−342.1	−342.3	−342.4	−338.3	−336.3	−340.5
54	37	−338.3	−340.4	−341.9	−329.5	−330.1	−342.6
55	37	−335.8	−338.6	−340.6	−326.2	−322.8	−337.2
56	23	−348.3	−351.9	−354.4	−336.7	−338.7	−356.5
57	26	−348.2	−351.7	−354.3	−335.4	−337.2	−356.2
58	26	−342.5	−345.7	−348.0	−331.2	−333.2	−350.0
59	29	−335.4	−338.8	−341.3	−322.4	−323.9	−342.8
60	29	−339.9	−343.0	−345.3	−328.9	−330.8	−347.3
61	32	−347.7	−351.9	−354.9	−336.0	−337.8	−356.7
62	32	−338.4	−341.6	−344.0	−329.4	−331.3	−345.8
63	40	−400.3	−406.0	−410.1	−384.3	−383.5	−409.2

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Table 2 – continued from previous page

N	n_{atom}	$E^{MP2}_{cc-pVTZ}$	$E^{MP2}_{cc-pVQZ}$	E^{MP2}_{CBS}	E^{MP2}_{small}	$E^{CCSD(T)}_{small}$	$E^{CCSD(T)}_{CBS}$
64	26	−366.5	−368.1	−369.4	−361.2	−361.7	−369.9
65	26	−359.6	−360.3	−360.8	−355.2	−355.4	−361.0
66	29	−363.2	−365.0	−366.3	−357.9	−358.5	−366.8
67	29	−349.5	−350.9	−351.9	−343.8	−344.1	−352.2
68	29	−355.7	−356.9	−357.7	−351.5	−351.9	−358.1
69	32	−362.5	−363.7	−364.6	−354.7	−355.1	−365.1
70	32	−347.2	−348.5	−349.5	−339.5	−339.9	−349.8
71	32	−354.6	−355.3	−355.8	−347.8	−348.1	−356.0
72	35	−360.7	−362.4	−363.6	−353.4	−353.9	−364.1
73	35	−345.9	−347.2	−348.2	−338.5	−338.9	−348.5
74	35	−353.4	−354.1	−354.6	−346.7	−346.9	−354.9
75	22	−401.8	−400.9	−400.2	−395.3	−393.4	−398.4
76	25	−401.5	−400.9	−400.5	−394.2	−392.0	−398.3
77	25	−386.9	−386.2	−385.6	−379.4	−377.2	−383.4
78	25	−396.4	−395.6	−395.0	−389.8	−388.0	−393.2
79	28	−399.8	−399.4	−399.1	−392.3	−390.1	−396.9
80	28	−383.7	−383.6	−383.4	−376.3	−374.5	−381.7
81	28	−394.5	−393.7	−393.1	−387.9	−385.9	−391.2
82	31	−398.2	−397.7	−397.3	−400.6	−399.2	−395.8
83	31	−383.2	−382.9	−382.7	−385.7	−384.1	−381.1
84	31	−392.6	−392.0	−391.6	−396.4	−395.0	−390.2
85	26	−351.3	−353.0	−354.2	−344.3	−341.0	−350.8
86	26	−357.9	−359.6	−360.9	−350.4	−346.4	−356.9
87	26	−337.8	−338.7	−339.3	−334.5	−331.0	−335.8
88	26	−357.0	−358.6	−359.8	−349.7	−346.0	−356.1
89	29	−346.7	−348.2	−349.2	−339.7	−336.2	−345.7
90	29	−350.4	−351.9	−352.9	−342.2	−338.0	−348.8
91	29	−346.7	−348.2	−349.2	−339.7	−336.1	−345.7
92	29	−350.3	−351.8	−353.0	−342.1	−338.0	−348.9
93	29	−353.4	−355.2	−356.4	−346.1	−342.0	−352.3
94	29	−353.4	−355.2	−356.5	−346.1	−342.0	−352.4
95	32	−347.6	−349.0	−350.1	−335.5	−332.5	−347.1
96	32	−347.9	−349.4	−350.5	−334.8	−331.4	−347.2

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Table 2 – continued from previous page

N	n_{atom}	$E^{MP2}_{cc-pVTZ}$	$E^{MP2}_{cc-pVQZ}$	E^{MP2}_{CBS}	E^{MP2}_{small}	$E^{CCSD(T)}_{small}$	$E^{CCSD(T)}_{CBS}$
97	32	−349.2	−350.9	−352.1	−337.2	−334.2	−349.1
98	32	−324.8	−325.3	−325.6	−319.5	−316.7	−322.8
99	32	−345.5	−347.2	−348.4	−333.7	−330.5	−345.3
100	32	−352.1	−353.9	−355.3	−340.3	−336.9	−351.9
101	35	−343.0	−344.4	−345.4	−331.6	−328.3	−342.1
102	35	−346.5	−347.8	−348.8	−333.7	−330.3	−345.4
103	35	−347.5	−349.1	−350.3	−334.9	−331.9	−347.2
104	35	−346.4	−347.9	−348.9	−333.7	−330.3	−345.5
105	35	−347.8	−349.3	−350.4	−336.5	−333.2	−347.2
106	35	−350.4	−352.1	−353.3	−338.6	−335.2	−349.9
107	29	−403.9	−405.1	−405.9	−397.1	−396.3	−405.1
108	29	−392.1	−392.1	−392.1	−387.9	−386.9	−391.2
109	32	−402.0	−403.0	−403.7	−393.7	−393.0	−403.1
110	32	−386.1	−386.9	−387.5	−377.2	−376.7	−386.9
111	32	−390.5	−390.7	−390.8	−384.3	−383.6	−390.0
112	35	−400.9	−402.1	−403.0	−392.6	−391.9	−402.3
113	35	−383.3	−384.3	−385.0	−374.6	−374.2	−384.5
114	35	−389.2	−389.7	−390.0	−383.2	−382.5	−389.3
115	38	−399.0	−400.4	−401.5	−391.0	−390.3	−400.8
116	38	−382.5	−383.1	−383.5	−373.8	−373.3	−383.0
117	38	−387.8	−388.3	−388.6	−381.8	−381.1	−387.9
118	36	−335.7	−335.1	−334.6	−333.6	−331.0	−332.1
119	36	−327.1	−327.6	−328.0	−323.9	−323.2	−327.3
120	36	−333.8	−333.0	−332.5	−332.7	−330.2	−330.0
121	36	−329.6	−329.9	−330.1	−325.5	−324.7	−329.4
122	39	−333.7	−333.7	−333.8	−331.3	−328.8	−331.2
123	39	−323.9	−324.5	−324.9	−320.3	−319.6	−324.2
124	39	−326.5	−325.9	−325.5	−324.1	−321.7	−323.1
125	39	−319.9	−320.7	−321.2	−314.4	−313.6	−320.4
126	39	−322.5	−322.9	−323.1	−318.3	−317.7	−322.5
127	42	−333.0	−332.9	−332.8	−330.2	−327.7	−330.3
128	28	−342.8	−343.9	−344.8	−337.1	−337.2	−344.8
129	28	−336.8	−337.1	−337.4	−331.5	−331.5	−337.3

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Table 2 – continued from previous page

N	n_{atom}	$E^{MP2}_{cc-pVTZ}$	$E^{MP2}_{cc-pVQZ}$	E^{MP2}_{CBS}	E^{MP2}_{small}	$E^{CCSD(T)}_{small}$	$E^{CCSD(T)}_{CBS}$
130	31	−337.2	−338.6	−339.6	−331.3	−331.4	−339.7
131	31	−326.3	−327.5	−328.3	−320.0	−320.1	−328.4
132	31	−332.9	−333.5	−334.0	−327.2	−327.3	−334.1
133	34	−339.3	−340.2	−340.9	−332.6	−332.8	−341.0
134	34	−324.2	−325.0	−325.7	−317.6	−317.8	−325.8
135	34	−331.8	−332.3	−332.6	−326.0	−326.1	−332.7
136	37	−337.5	−338.8	−339.8	−331.3	−331.4	−340.0
137	37	−323.3	−324.1	−324.6	−316.8	−317.0	−324.8
138	37	−330.7	−331.3	−331.8	−325.0	−325.1	−332.0
139	39	−392.5	−394.5	−395.9	−384.5	−384.1	−395.5
140	45	−389.5	−391.7	−393.3	−381.3	−380.8	−392.8
141	45	−372.5	−373.9	−374.9	−363.4	−363.2	−374.7
142	25	−481.1	−478.1	−476.0	−480.5	−479.4	−474.9
143	21	−496.1	−493.3	−491.2	−495.0	−494.4	−490.6
144	18	−509.1	−506.1	−503.9	−495.4	−495.8	−504.3
145	25	−463.5	−460.4	−458.2	−464.1	−463.2	−457.3
146	21	−477.4	−474.4	−472.3	−477.6	−476.9	−471.7
147	18	−492.6	−489.6	−487.4	−479.7	−480.2	−487.9
148	14	−447.1	−444.5	−442.5	−428.8	−425.5	−439.2
149	14	−426.2	−427.8	−429.0	−412.1	−415.4	−432.3
150	17	−442.1	−439.6	−437.7	−427.9	−427.1	−437.0
151	17	−396.1	−399.4	−401.8	−392.5	−390.6	−399.9
152	18	−362.5	−363.0	−363.5	−355.3	−356.6	−364.7
153	18	−359.1	−362.6	−365.1	−357.5	−356.1	−363.7
154	21	−441.1	−440.5	−440.1	−438.1	−437.4	−439.3
155	21	−361.3	−362.3	−363.1	−355.4	−356.9	−364.6
156	21	−397.3	−400.2	−402.3	−387.1	−387.9	−403.1
157	21	−376.9	−378.5	−379.6	−370.4	−371.0	−380.1
158	17	−442.4	−439.6	−437.6	−424.2	−421.1	−434.6
159	17	−441.9	−439.2	−437.2	−423.7	−420.6	−434.1
160	20	−437.5	−434.9	−433.0	−423.4	−422.8	−432.4
161	20	−404.1	−407.4	−409.9	−400.7	−398.1	−407.2
162	21	−392.6	−391.9	−391.4	−391.2	−389.1	−389.4

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Table 2 – continued from previous page

N	n_{atom}	$E^{MP2}_{cc-pVTZ}$	$E^{MP2}_{cc-pVQZ}$	E^{MP2}_{CBS}	E^{MP2}_{small}	$E^{CCSD(T)}_{small}$	$E^{CCSD(T)}_{CBS}$
163	21	−376.0	−378.6	−380.6	−365.7	−364.8	−379.6
164	24	−426.0	−424.8	−423.9	−424.2	−421.2	−420.9
165	24	−386.9	−385.5	−384.5	−384.3	−381.6	−381.7
166	24	−430.7	−433.2	−435.1	−420.4	−420.0	−434.7
167	24	−388.2	−388.9	−389.4	−383.8	−383.7	−389.3
168	20	−441.1	−438.3	−436.3	−423.0	−419.9	−433.2
169	20	−441.5	−439.0	−437.1	−423.6	−420.5	−434.0
170	23	−428.2	−425.4	−423.3	−428.0	−424.4	−419.7
171	23	−430.8	−430.5	−430.2	−425.7	−424.1	−428.6
172	24	−394.3	−394.6	−394.7	−388.9	−387.7	−393.5
173	24	−362.0	−365.1	−367.3	−353.2	−354.2	−368.3
174	27	−385.5	−383.9	−382.7	−383.8	−380.8	−379.8
175	27	−441.5	−443.5	−445.0	−432.0	−431.2	−444.2
176	27	−390.3	−391.8	−393.0	−381.4	−380.3	−391.9
177	23	−439.3	−436.5	−434.5	−438.0	−435.2	−431.8
178	23	−405.7	−408.6	−410.7	−391.9	−395.5	−414.3
179	26	−426.9	−424.1	−422.1	−426.7	−423.2	−418.6
180	26	−434.6	−432.0	−430.0	−434.9	−433.2	−428.4
181	27	−396.8	−398.2	−399.3	−389.2	−387.4	−397.5
182	27	−395.1	−397.0	−398.4	−386.9	−385.1	−396.7
183	30	−423.2	−422.0	−421.1	−418.7	−416.0	−418.5
184	30	−384.2	−382.6	−381.3	−378.5	−375.9	−378.7
185	30	−440.1	−441.5	−442.5	−430.8	−430.2	−441.8
186	30	−392.1	−392.3	−392.5	−382.2	−381.3	−391.6
187	19	−483.3	−481.4	−480.0	−466.3	−462.2	−475.9
188	22	−464.3	−462.5	−461.2	−461.3	−458.4	−458.3
189	23	−426.5	−426.8	−427.0	−418.0	−414.5	−423.5
190	26	−467.8	−467.9	−467.9	−461.4	−459.1	−465.6
191	26	−419.4	−418.5	−417.8	−414.8	−412.5	−415.5
192	22	−478.1	−476.7	−475.6	−471.5	−467.6	−471.7
193	25	−458.7	−456.7	−455.2	−455.5	−452.3	−452.0
194	26	−419.5	−420.0	−420.4	−411.1	−407.2	−416.5
195	29	−463.7	−463.3	−463.1	−456.9	−454.1	−460.3

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Table 2 – continued from previous page

N	n_{atom}	$E^{MP2}_{cc-pVTZ}$	$E^{MP2}_{cc-pVQZ}$	E^{MP2}_{CBS}	E^{MP2}_{small}	$E^{CCSD(T)}_{small}$	$E^{CCSD(T)}_{CBS}$
196	29	−413.6	−412.3	−411.4	−408.2	−405.4	−408.6
197	25	−409.4	−409.7	−410.0	−399.5	−397.0	−407.5
198	28	−390.6	−390.9	−391.1	−383.8	−381.7	−389.0
199	29	−366.9	−369.1	−370.8	−357.4	−355.3	−368.7
200	32	−406.8	−409.0	−410.7	−394.5	−393.6	−409.8
201	32	−363.1	−364.0	−364.5	−353.5	−352.2	−363.3
202	18	−481.5	−479.3	−477.7	−463.8	−460.4	−474.2
203	21	−467.0	−464.6	−462.8	−464.1	−461.6	−460.3
204	22	−423.5	−423.0	−422.6	−418.4	−415.3	−419.5
205	25	−467.6	−466.9	−466.3	−462.9	−461.1	−464.5
206	25	−414.2	−412.4	−411.2	−411.2	−409.6	−409.6
207	21	−397.1	−397.0	−397.0	−387.1	−385.0	−395.0
208	24	−378.6	−379.0	−379.3	−371.7	−370.4	−378.1
209	25	−357.6	−359.4	−360.7	−349.1	−347.5	−359.1
210	28	−392.8	−394.2	−395.3	−384.2	−383.5	−394.6
211	28	−348.3	−349.5	−350.4	−340.2	−339.9	−350.1
212	15	−487.8	−485.0	−483.0	−468.8	−466.2	−480.4
213	18	−477.6	−474.8	−472.7	−462.4	−461.6	−472.0
214	19	−436.7	−437.3	−437.7	−427.3	−425.8	−436.2
215	22	−480.2	−479.9	−479.6	−477.2	−476.3	−478.6
216	22	−437.4	−435.7	−434.6	−433.9	−432.3	−432.9
217	18	−485.4	−483.4	−481.9	−467.1	−464.2	−478.9
218	21	−475.2	−472.7	−470.8	−472.6	−470.5	−468.6
219	22	−434.9	−435.3	−435.6	−426.3	−423.5	−432.8
220	25	−471.5	−470.9	−470.5	−466.9	−465.0	−468.6
221	25	−435.4	−434.4	−433.7	−431.6	−430.0	−432.2
222	21	−401.2	−402.3	−403.2	−388.6	−386.5	−401.0
223	24	−467.2	−464.6	−462.7	−465.1	−463.0	−460.6
224	25	−361.9	−364.2	−365.9	−352.6	−350.6	−364.0
225	28	−468.2	−466.9	−465.9	−465.3	−463.8	−464.5
226	28	−421.6	−420.5	−419.6	−417.5	−415.9	−418.0
227	12	−500.9	−498.4	−496.6	−481.3	−478.9	−494.3
228	15	−472.8	−470.5	−468.8	−460.2	−461.0	−469.6

Continued on next page

Table 2 – continued from previous page

N	n_{atom}	$E^{MP2}_{cc-pVTZ}$	$E^{MP2}_{cc-pVQZ}$	E^{MP2}_{CBS}	E^{MP2}_{small}	$E^{CCSD(T)}_{small}$	$E^{CCSD(T)}_{CBS}$
229	16	−447.9	−447.3	−446.9	−438.2	−436.1	−444.8
230	19	−465.6	−464.2	−463.3	−455.9	−455.3	−462.7
231	19	−429.9	−428.0	−426.7	−419.0	−418.8	−426.6
232	15	−492.7	−490.5	−488.8	−474.1	−472.0	−486.7
233	18	−479.5	−477.3	−475.6	−465.3	−464.9	−475.3
234	19	−443.6	−444.1	−444.6	−434.1	−432.4	−442.8
235	22	−479.4	−479.5	−479.5	−476.3	−475.7	−479.0
236	22	−437.1	−435.6	−434.5	−434.4	−433.0	−433.0

Table 3: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the BLYP functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−23.7	29.3	−6.6	31.3	31.6	37.0	−18.6	29.5	26.9	35.2
2	−29.0	30.5	−9.3	32.8	32.9	38.9	−22.1	31.9	27.9	37.1
3	−25.8	27.4	−8.7	29.3	30.6	36.1	−20.3	28.2	25.8	34.1
4	−29.6	31.9	−9.8	34.0	34.1	40.2	−22.9	33.3	29.0	38.5
5	−27.7	30.0	−9.5	31.8	32.6	38.6	−22.0	30.6	27.5	36.6
6	−29.6	32.5	−9.9	34.6	34.6	40.9	−23.2	33.8	29.5	39.1
7	−27.4	30.2	−9.2	32.0	33.0	38.8	−21.9	30.8	28.0	36.8
8	−9.2	15.4	19.1	26.4	20.3	24.7	−88.1	−5.1	−10.6	11.7
9	−8.2	18.0	20.7	28.4	22.3	27.0	−89.5	−0.4	−9.2	14.5
10	−17.3	0.4	14.7	20.3	16.9	20.4	−87.0	−17.1	−13.5	4.4
11	−14.9	3.6	15.8	21.7	18.6	22.2	−86.9	−13.2	−11.9	6.5
12	−8.3	16.4	19.7	27.1	21.2	25.8	−87.9	−4.1	−9.7	12.9
13	−6.2	20.3	22.5	30.4	24.2	29.0	−87.9	1.6	−7.3	16.6
14	−16.7	1.0	15.0	20.7	17.2	20.8	−86.8	−16.7	−13.1	4.9
15	−12.3	9.0	18.9	25.3	21.9	25.8	−87.3	−5.9	−9.3	11.2
16	−5.2	21.8	23.2	31.1	25.0	29.8	−87.3	1.4	−6.7	17.4
17	−5.6	21.0	23.1	31.3	25.0	29.7	−87.6	2.3	−6.7	17.5
18	−15.8	2.5	15.9	22.2	18.3	22.0	−86.3	−15.1	−12.3	6.6

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Table 3 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
19	−11.3	10.9	19.8	26.7	22.8	26.9	−87.2	−3.7	−8.5	12.9
20	−4.7	22.4	23.7	31.7	25.5	30.4	−87.1	2.0	−6.1	18.1
21	14.3	38.9	22.1	40.3	44.5	46.2	9.5	38.2	39.1	43.4
22	−5.1	12.5	4.8	19.5	27.6	28.6	−6.6	16.5	22.7	25.5
23	16.1	41.2	24.2	43.0	47.8	49.5	11.8	40.3	42.0	46.5
24	13.4	38.7	21.6	40.5	44.9	46.3	8.7	37.9	39.1	43.5
25	13.2	39.7	21.7	41.4	45.6	47.2	8.2	38.8	39.9	44.6
26	13.4	37.7	21.2	39.2	43.9	45.5	8.9	36.7	38.4	42.7
27	14.0	38.7	21.8	39.8	44.4	46.1	9.1	37.7	38.9	43.3
28	16.5	41.2	24.0	42.2	46.2	48.0	11.8	40.1	40.9	45.3
29	16.8	42.2	24.8	43.8	48.5	50.2	12.5	41.1	42.8	47.3
30	16.5	44.5	25.3	45.5	49.4	51.2	12.0	43.1	43.7	48.6
31	3.9	26.1	13.8	31.1	38.6	39.8	1.6	29.0	32.8	36.6
32	15.4	44.2	24.3	45.4	49.3	51.1	10.7	43.3	43.4	48.5
33	18.2	43.0	25.5	43.7	47.9	49.9	13.4	41.3	42.6	47.2
34	17.5	42.2	24.8	42.9	46.9	48.7	12.5	40.6	41.6	46.1
35	18.2	43.8	26.3	45.5	50.2	52.0	13.8	42.7	44.4	49.1
36	18.1	47.5	27.0	48.6	52.3	54.2	13.2	46.5	46.4	51.7
37	20.0	44.7	27.2	45.4	49.5	51.6	15.1	42.9	44.3	48.9
38	7.1	43.1	18.9	42.5	43.6	48.4	−22.4	37.4	33.7	44.1
39	7.4	45.1	21.8	45.9	45.8	51.0	−25.7	40.8	35.3	46.7
40	7.3	43.7	19.3	43.2	44.5	49.6	−22.8	37.7	34.7	45.4
41	8.1	48.0	22.9	48.8	48.5	53.8	−26.1	43.7	37.7	49.5
42	8.1	44.6	19.9	43.9	45.4	50.5	−22.5	38.2	35.6	46.3
43	9.0	49.7	23.9	50.3	49.8	55.3	−25.6	45.2	38.9	51.1
44	8.1	44.7	19.8	43.9	45.4	50.5	−22.6	38.2	35.7	46.4
45	15.7	49.9	26.6	52.9	55.4	62.7	−5.7	44.2	51.7	58.7
46	−8.7	7.8	−1.1	15.5	25.4	29.1	−25.2	6.2	21.0	25.1
47	5.8	34.4	16.7	36.5	40.5	46.1	−9.9	29.5	37.1	42.6
48	16.3	55.6	28.8	59.5	61.0	69.4	−5.7	50.3	57.7	65.5
49	−7.4	19.1	3.9	26.7	35.2	40.1	−23.4	17.4	30.7	36.0
50	4.5	36.3	17.4	38.7	42.8	49.0	−12.8	32.0	39.4	45.3

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Table 3 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
51	14.8	49.0	26.4	51.6	54.9	62.0	−5.2	43.6	51.3	57.8
52	17.5	59.0	30.8	62.8	63.8	72.7	−4.3	53.8	60.6	68.9
53	−5.8	23.6	6.4	30.5	38.9	44.2	−22.6	22.0	34.2	40.0
54	4.5	38.1	18.2	40.3	44.4	50.8	−12.7	33.8	40.9	47.1
55	15.9	50.6	27.6	52.9	55.3	62.4	−3.0	44.7	52.0	58.4
56	−14.4	33.1	6.1	35.9	32.3	38.3	−24.7	27.9	27.0	35.7
57	−18.8	36.4	4.4	39.6	34.9	41.8	−28.8	31.8	29.7	39.2
58	−14.5	33.1	5.7	35.6	32.2	38.5	−24.7	27.8	27.1	35.8
59	−16.0	36.8	4.6	38.3	33.3	40.3	−28.8	30.8	28.3	37.9
60	−14.3	33.2	5.6	35.6	32.3	38.7	−24.8	27.7	27.2	36.0
61	−18.8	39.9	5.1	42.9	37.8	45.3	−29.5	35.3	32.4	42.8
62	−14.2	33.3	5.8	35.7	32.4	38.8	−24.8	27.8	27.4	36.1
63	19.7	56.5	32.1	55.9	53.4	58.5	−12.1	53.8	45.6	56.3
64	−47.9	6.4	−26.0	13.8	21.6	25.8	−37.2	13.8	15.7	23.2
65	−46.8	0.3	−26.6	8.5	17.1	21.0	−35.5	8.8	11.7	18.5
66	−46.9	8.1	−25.6	15.0	22.7	27.1	−37.0	15.0	16.8	24.6
67	−45.0	6.3	−25.7	13.1	19.5	23.8	−35.9	13.2	14.3	21.7
68	−46.1	1.9	−26.3	9.7	18.2	22.4	−35.4	10.0	12.8	19.9
69	−46.9	9.0	−26.2	15.6	22.9	27.5	−37.6	15.5	16.9	25.0
70	−45.7	6.2	−26.2	12.9	19.4	23.9	−36.8	13.0	14.3	21.8
71	−45.9	2.3	−26.6	9.9	18.2	22.6	−35.8	10.1	12.9	20.1
72	−46.2	9.6	−25.6	16.2	23.5	28.1	−37.2	16.1	17.6	25.7
73	−45.1	6.7	−25.8	13.4	19.9	24.5	−36.5	13.3	14.8	22.4
74	−45.8	2.6	−26.5	10.2	18.5	22.9	−35.8	10.3	13.2	20.4
75	−18.4	0.1	13.5	19.1	17.1	20.6	−94.0	−18.3	−13.4	4.0
76	−15.2	5.1	15.8	22.3	19.7	23.6	−91.6	−13.9	−11.2	8.0
77	−16.5	3.8	13.4	19.7	17.2	21.0	−90.7	−14.1	−12.8	6.0
78	−16.9	1.8	14.4	20.1	18.1	21.6	−92.5	−16.7	−12.2	5.4
79	−14.6	6.6	16.3	23.4	20.4	24.5	−91.3	−12.3	−10.8	9.4
80	−14.9	5.5	14.7	21.0	18.5	22.3	−89.0	−12.5	−11.3	7.6
81	−16.6	2.8	14.6	20.8	18.4	22.1	−92.3	−15.7	−12.1	6.3
82	−13.7	7.5	17.2	24.2	21.2	25.3	−90.5	−11.4	−9.9	10.4

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Table 3 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
83	−14.8	5.7	15.2	21.9	19.1	23.0	−89.7	−12.7	−11.0	8.3
84	−15.6	3.8	15.4	21.7	19.2	23.1	−91.4	−14.8	−11.1	7.4
85	−9.2	13.8	1.1	18.0	26.2	26.7	−13.0	15.9	19.9	23.4
86	−4.4	17.8	5.8	22.1	30.3	30.9	−7.6	19.8	24.1	27.6
87	1.6	19.0	8.8	21.9	32.4	33.0	−1.4	19.4	26.6	29.7
88	−4.1	16.9	5.8	21.1	29.8	30.3	−6.8	18.7	23.7	27.0
89	−8.4	14.7	1.4	18.4	26.4	27.0	−12.5	16.3	20.1	23.7
90	−4.0	19.1	6.1	22.8	30.3	31.0	−6.8	20.8	24.2	27.8
91	−8.5	14.8	1.3	18.5	26.3	27.0	−12.6	16.4	20.0	23.8
92	−3.9	19.2	6.2	22.9	30.4	31.1	−6.6	20.9	24.2	28.0
93	−3.5	18.9	6.4	22.8	31.0	31.6	−7.0	20.5	24.8	28.4
94	−3.3	18.9	6.5	22.8	31.2	31.7	−6.9	20.5	25.0	28.4
95	−4.7	19.3	4.1	22.2	29.4	30.0	−9.2	20.3	22.9	26.9
96	−2.9	20.3	7.2	23.9	31.4	32.1	−5.7	21.9	25.2	29.0
97	−4.6	19.7	4.2	22.7	29.7	30.4	−9.2	20.9	23.1	27.2
98	4.1	21.7	10.4	23.6	33.4	34.2	0.5	21.6	27.8	31.0
99	−1.7	20.3	7.3	23.7	30.9	31.7	−5.5	21.3	24.8	28.6
100	−2.1	20.4	7.5	24.2	32.4	33.0	−6.0	21.8	26.0	29.7
101	2.0	21.2	9.8	24.6	31.7	32.3	−1.6	21.5	25.8	29.4
102	−3.0	20.1	7.1	23.8	31.5	32.2	−6.0	21.6	25.3	29.1
103	−3.6	21.4	5.4	24.1	30.7	31.6	−7.9	22.4	24.2	28.5
104	−2.8	20.1	7.3	23.9	31.7	32.2	−5.8	21.6	25.5	29.1
105	−1.2	19.9	8.4	23.8	32.1	32.8	−4.2	21.2	26.2	29.6
106	−1.8	20.5	7.8	24.3	32.7	33.1	−5.7	21.9	26.3	29.9
107	−11.3	19.0	4.5	26.4	31.5	35.1	−41.3	18.1	20.7	29.9
108	−15.9	7.4	−0.8	17.5	23.5	26.4	−43.6	7.4	13.7	21.1
109	−10.1	22.0	5.7	29.0	33.5	37.5	−40.6	20.4	22.6	32.3
110	−10.2	20.6	4.4	26.6	30.4	34.2	−38.3	19.1	20.1	29.5
111	−13.4	11.6	1.1	20.9	26.2	29.6	−42.4	11.0	16.4	24.4
112	−8.6	24.3	7.2	31.2	35.3	39.2	−39.7	22.4	24.2	34.2
113	−9.6	21.1	5.1	27.1	31.0	34.7	−37.8	19.5	20.8	30.1
114	−12.6	13.6	1.9	22.5	27.6	31.1	−42.1	12.7	17.4	26.1

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Table 3 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
115	−8.2	24.7	7.5	31.5	35.7	39.6	−39.3	22.7	24.6	34.6
116	−9.2	21.4	5.3	27.5	31.5	35.1	−37.8	19.6	21.3	30.5
117	−12.4	14.1	2.1	22.8	27.8	31.5	−42.0	13.0	17.7	26.5
118	−3.5	19.2	4.8	24.6	33.4	37.5	−21.7	16.6	28.5	33.4
119	−2.9	20.4	5.4	22.9	29.0	33.6	−19.6	15.8	25.4	29.7
120	−6.0	14.3	1.4	20.6	30.2	34.3	−23.9	12.4	25.4	30.1
121	−4.3	20.6	5.5	23.4	29.8	34.2	−21.0	16.8	25.8	30.3
122	−0.1	23.8	7.7	28.6	36.3	41.1	−19.8	21.0	31.5	36.9
123	−2.9	22.7	5.7	25.3	31.1	35.8	−19.8	17.7	27.6	32.1
124	−3.6	20.0	4.7	24.9	34.0	38.3	−24.0	17.7	29.1	34.3
125	−2.4	25.2	7.1	27.2	32.6	37.2	−18.9	20.7	28.7	33.6
126	−3.4	22.4	5.8	24.6	30.4	35.1	−19.9	18.0	26.7	31.3
127	−0.9	25.3	8.6	30.0	38.1	42.8	−20.5	22.5	33.0	38.5
128	−34.6	11.5	−9.8	18.8	20.8	25.4	−41.4	11.2	14.5	22.2
129	−35.2	6.7	−11.6	14.7	16.7	21.1	−40.9	7.2	10.9	17.9
130	−33.4	12.6	−9.6	19.5	21.0	26.2	−40.8	12.0	15.0	23.0
131	−33.0	11.3	−10.7	18.0	19.2	24.1	−40.0	11.0	13.6	21.3
132	−34.0	8.3	−10.9	15.8	17.8	22.5	−40.2	8.5	12.1	19.3
133	−33.2	14.6	−9.1	21.2	22.5	28.0	−41.1	13.7	16.2	24.8
134	−33.0	11.3	−10.7	17.9	19.0	24.0	−40.1	10.9	13.5	21.3
135	−33.5	9.1	−10.9	16.5	18.1	23.2	−40.3	9.1	12.4	20.1
136	−32.7	15.1	−8.6	21.7	23.0	28.4	−40.8	14.2	16.7	25.2
137	−32.4	11.9	−10.2	18.5	19.6	24.7	−39.7	11.4	14.2	22.0
138	−33.1	9.9	−10.5	17.2	18.7	23.9	−40.1	9.7	13.0	20.8
139	−2.6	24.2	11.8	30.2	33.6	37.0	−30.1	24.8	25.6	33.8
140	0.0	29.4	14.3	35.0	37.4	41.3	−28.4	29.2	29.1	38.2
141	−1.0	26.1	12.1	30.8	33.0	36.4	−27.4	25.8	25.5	33.6
142	−43.0	−7.8	−28.4	2.5	19.4	21.1	−45.1	−4.2	6.1	14.1
143	−40.7	−8.8	−27.2	1.5	18.3	20.1	−41.5	−4.0	5.2	12.8
144	−39.9	−9.5	−27.1	1.4	18.5	20.3	−40.9	−4.2	5.6	13.0
145	−44.4	−10.9	−29.4	−0.2	17.3	18.9	−46.1	−7.2	5.0	12.4
146	−42.3	−12.0	−28.6	−1.3	16.1	17.7	−43.0	−7.1	3.8	10.7

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Table 3 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
147	−42.8	−12.7	−28.4	−1.0	16.8	18.6	−42.9	−6.9	4.6	11.6
148	−15.5	−4.6	13.1	17.2	14.5	17.2	−74.1	−25.2	−13.4	−0.7
149	−19.2	2.0	10.0	16.5	10.6	14.6	−97.2	−26.1	−20.4	−0.7
150	−37.3	−6.5	−25.8	2.3	18.6	21.1	−42.4	−2.5	6.3	13.6
151	−12.6	25.1	−10.6	26.7	33.0	37.7	−25.4	22.8	21.5	32.1
152	−10.7	8.2	0.0	16.7	18.3	21.5	−31.7	5.9	11.7	17.3
153	3.1	28.3	8.5	28.3	27.1	31.4	−22.8	17.9	20.6	27.6
154	−15.3	3.8	2.0	17.2	22.3	25.0	−34.2	4.7	12.7	19.1
155	−8.6	16.4	3.3	23.3	26.7	30.2	−28.3	13.9	19.9	26.0
156	2.3	28.0	14.1	32.1	32.0	35.8	−24.0	23.7	23.5	31.7
157	−5.0	22.6	4.8	26.0	30.3	34.3	−25.9	17.7	23.1	29.6
158	−15.3	−4.3	13.0	17.1	15.1	17.9	−73.9	−24.8	−12.9	−0.1
159	−15.5	−4.5	12.8	16.9	14.9	17.5	−74.4	−25.3	−13.3	−0.5
160	−36.8	−6.1	−25.6	2.5	19.2	21.7	−42.2	−2.4	6.8	14.0
161	−9.0	29.7	−7.5	30.6	36.8	41.4	−20.2	28.6	24.9	35.8
162	−14.5	2.1	−2.5	13.5	17.0	19.8	−31.1	−0.5	9.8	14.4
163	4.0	30.8	11.5	32.7	32.0	36.9	−22.4	23.6	25.3	32.7
164	−18.5	0.9	−2.5	13.8	19.6	21.8	−33.8	1.8	10.2	16.0
165	−14.2	2.8	−0.7	15.0	19.3	21.9	−30.9	1.6	11.8	16.5
166	−2.2	28.3	12.7	32.9	35.3	39.5	−30.0	24.6	25.3	34.7
167	−13.2	13.9	0.9	22.1	26.9	30.5	−33.3	9.9	19.4	25.6
168	−15.1	−4.1	13.3	17.4	15.6	18.4	−73.9	−24.5	−12.4	0.4
169	−15.2	−3.9	13.2	17.5	15.6	18.3	−74.7	−24.5	−12.6	0.3
170	−37.7	−7.5	−26.3	1.3	17.2	19.9	−42.4	−3.6	5.1	12.3
171	−36.8	2.2	−28.4	8.4	21.8	25.4	−46.8	2.9	8.3	18.4
172	−9.6	9.2	4.0	21.3	22.2	25.8	−32.3	6.4	14.7	20.5
173	−3.0	26.9	7.1	31.1	31.0	35.7	−31.1	22.0	23.5	31.7
174	−15.1	1.4	−1.7	14.0	18.7	21.4	−31.5	0.7	11.5	16.0
175	−9.7	23.6	8.2	30.9	34.1	38.4	−37.7	21.6	23.5	33.5
176	−7.9	21.7	7.7	28.7	32.6	37.3	−32.4	21.4	24.5	33.2
177	−14.6	−3.6	13.7	17.8	16.0	18.8	−73.1	−24.1	−11.9	0.9
178	−13.4	13.3	15.9	23.8	17.9	22.6	−96.2	−9.2	−13.8	9.8

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Table 3 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
179	−37.4	−7.2	−26.0	1.6	17.6	20.3	−42.1	−3.3	5.5	12.6
180	−37.5	−6.7	−26.4	1.7	18.6	21.2	−43.0	−3.2	6.2	13.5
181	−8.3	17.6	4.8	27.0	27.3	31.9	−34.7	13.9	19.8	27.2
182	−6.9	20.1	5.9	28.8	28.8	33.6	−33.9	16.4	21.5	29.1
183	−17.2	2.1	−1.3	14.9	20.8	23.0	−32.5	2.7	11.4	17.2
184	−14.6	1.8	−1.2	14.3	19.1	21.8	−30.9	1.1	11.8	16.4
185	−9.6	19.7	7.7	29.1	32.6	36.5	−36.7	18.5	22.2	31.5
186	−11.5	12.9	4.0	23.4	27.9	31.9	−33.8	13.7	19.8	27.6
187	−16.6	3.7	15.8	22.2	18.5	22.4	−91.3	−19.2	−13.6	5.6
188	−37.3	4.7	−27.5	10.5	25.1	28.8	−48.2	3.4	11.2	21.2
189	−10.4	17.9	4.2	28.7	28.8	33.3	−38.5	12.8	20.2	27.9
190	−14.3	16.7	4.6	27.5	32.0	35.7	−43.1	14.1	20.4	29.8
191	−15.4	10.6	1.2	22.3	27.5	31.2	−39.7	9.2	18.1	26.1
192	−14.8	8.7	18.6	25.9	21.6	26.0	−93.0	−12.9	−11.3	10.1
193	−38.6	4.9	−29.2	10.8	25.1	28.9	−50.2	4.2	10.9	21.5
194	−10.3	19.9	4.7	30.7	30.1	35.2	−39.7	14.6	21.7	29.9
195	−15.0	17.9	5.5	29.2	33.2	37.2	−45.2	15.4	21.5	31.5
196	−16.3	11.4	1.8	23.8	28.7	32.7	−41.9	10.7	19.3	27.7
197	−11.5	12.6	20.3	27.4	24.3	28.5	−91.7	−3.4	−7.6	14.1
198	−30.0	19.0	−24.2	19.2	30.4	34.3	−41.7	18.2	16.9	28.3
199	−2.6	30.9	7.2	35.1	35.6	40.6	−32.7	26.5	27.4	36.2
200	−3.0	34.9	12.6	39.0	41.5	45.9	−35.2	32.7	30.2	41.0
201	−9.6	28.7	4.7	33.7	37.8	42.5	−32.3	26.1	29.5	37.8
202	−16.0	1.7	14.0	20.1	16.2	19.9	−82.6	−22.2	−15.0	2.6
203	−42.2	−3.1	−31.8	4.2	20.2	23.5	−50.3	−1.5	6.2	15.5
204	−15.5	7.3	−2.0	18.6	21.0	24.7	−37.3	2.8	12.6	18.9
205	−17.4	7.4	0.8	20.1	25.5	28.5	−41.2	6.1	14.4	22.3
206	−20.3	0.2	−3.4	13.9	20.5	23.4	−40.9	0.3	11.6	18.1
207	−15.1	6.3	15.9	22.2	18.7	22.6	−89.9	−9.7	−11.5	7.6
208	−29.5	14.3	−23.4	14.9	25.7	29.2	−38.2	14.8	13.2	23.2
209	−7.0	20.8	4.3	27.3	28.1	32.2	−34.2	18.0	20.8	28.0
210	−9.4	21.2	5.9	27.7	31.3	34.9	−37.4	20.6	21.3	30.2

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Table 3 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
211	−4.9	20.6	6.6	25.6	29.4	33.0	−26.8	21.1	21.7	29.4
212	−17.7	−2.3	11.7	17.1	13.9	16.9	−82.9	−25.9	−16.8	−1.2
213	−41.9	−7.3	−31.6	1.2	18.4	21.4	−49.3	−4.9	4.7	13.1
214	−14.2	10.0	1.9	22.7	24.1	28.1	−39.4	7.1	15.8	22.5
215	−20.2	1.7	−0.9	16.3	23.1	26.0	−43.1	1.6	12.5	19.5
216	−20.5	2.3	−3.3	16.3	21.8	24.9	−40.1	0.3	13.3	18.7
217	−17.1	1.0	14.4	20.4	16.5	19.9	−87.9	−21.2	−15.1	2.2
218	−43.8	−4.5	−33.3	3.5	19.7	23.3	−52.4	−2.4	5.5	15.1
219	−11.8	15.1	3.8	27.0	27.3	31.7	−38.8	11.9	18.6	26.0
220	−16.7	10.2	1.3	23.0	27.7	30.7	−40.0	8.2	16.6	24.4
221	−21.6	7.3	−2.9	20.6	26.6	30.2	−40.8	5.8	17.7	24.2
222	−10.1	16.2	20.7	27.9	24.8	28.9	−88.0	4.3	−7.1	15.2
223	−42.2	−3.2	−32.3	4.4	20.7	24.4	−51.5	−1.7	6.6	16.2
224	−6.6	24.8	3.9	29.3	31.3	35.7	−35.4	22.2	23.1	31.5
225	−17.1	6.7	0.0	19.2	25.2	28.0	−38.3	4.5	14.3	21.5
226	−16.9	7.8	0.1	20.6	26.6	30.3	−41.1	7.7	16.9	24.8
227	−19.1	−3.3	11.7	16.8	13.0	16.0	−88.1	−25.1	−17.6	−2.1
228	−41.9	−12.3	−32.3	−4.1	12.7	15.2	−47.4	−9.0	0.5	7.5
229	−19.0	3.2	−5.3	14.3	17.0	20.0	−40.8	0.2	8.3	14.5
230	−21.3	−1.1	−7.1	9.6	15.2	17.1	−35.4	−1.5	5.8	11.9
231	−20.4	−5.0	−1.9	10.7	16.4	19.2	−36.8	−2.6	8.6	13.9
232	−17.6	−1.2	13.1	18.3	14.8	17.8	−87.8	−22.7	−15.9	0.0
233	−40.7	−3.1	−30.2	4.5	20.5	23.8	−48.7	−0.7	7.2	16.0
234	−10.8	14.9	4.4	26.7	26.7	30.8	−37.7	12.2	18.3	25.3
235	−20.4	5.5	−3.3	17.8	24.6	27.2	−42.7	4.5	13.8	21.2
236	−19.0	1.6	−3.8	14.6	19.1	22.2	−36.3	−0.9	11.4	16.2
MAXD	−47.9	59.0	−33.3	62.8	63.8	72.7	−97.2	53.8	60.6	68.9
MD	−13.2	16.7	3.3	24.5	28.4	32.0	−36.8	12.8	16.7	25.8
MAD	16.8	18.1	13.0	24.6	28.4	32.0	38.3	18.2	20.8	25.8

Table 4: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the BLYP-D3 functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−57.5	−4.5	−40.4	−2.5	−2.2	3.2	−52.4	−4.3	−6.9	1.4
2	−66.1	−6.6	−46.5	−4.4	−4.2	1.7	−59.3	−5.2	−9.2	−0.1
3	−59.0	−5.8	−41.9	−3.8	−2.6	2.9	−53.5	−5.0	−7.3	1.0
4	−67.9	−6.4	−48.1	−4.3	−4.3	1.9	−61.3	−5.1	−9.4	0.1
5	−63.7	−6.1	−45.6	−4.3	−3.5	2.5	−58.1	−5.4	−8.6	0.5
6	−68.7	−6.5	−48.9	−4.4	−4.4	1.9	−62.3	−5.2	−9.6	0.1
7	−63.7	−6.1	−45.6	−4.4	−3.3	2.4	−58.3	−5.6	−8.4	0.5
8	−28.6	−4.1	−0.3	6.9	0.8	5.2	−107.6	−24.6	−30.1	−7.7
9	−28.8	−2.6	0.1	7.8	1.7	6.4	−110.2	−21.0	−29.8	−6.2
10	−29.7	−12.1	2.2	7.8	4.5	8.0	−99.5	−29.6	−25.9	−8.0
11	−28.1	−9.7	2.5	8.4	5.3	8.9	−100.2	−26.5	−25.2	−6.7
12	−28.2	−3.4	−0.1	7.2	1.4	5.9	−107.8	−24.0	−29.5	−7.0
13	−27.3	−0.8	1.4	9.4	3.1	8.0	−109.0	−19.5	−28.3	−4.4
14	−29.5	−11.7	2.2	7.9	4.4	8.1	−99.6	−29.5	−25.9	−7.9
15	−28.1	−6.8	3.0	9.5	6.0	10.0	−103.2	−21.8	−25.2	−4.7
16	−27.6	−0.6	0.8	8.7	2.6	7.4	−109.6	−20.9	−29.0	−5.0
17	−27.1	−0.4	1.6	9.8	3.5	8.3	−109.0	−19.1	−28.1	−3.9
18	−29.3	−10.9	2.5	8.8	4.9	8.6	−99.7	−28.6	−25.7	−6.9
19	−28.3	−6.1	2.8	9.7	5.8	9.9	−104.2	−20.7	−25.6	−4.2
20	−27.5	−0.3	1.0	9.0	2.8	7.7	−109.9	−20.8	−28.8	−4.7
21	−24.6	0.1	−16.7	1.5	5.6	7.4	−29.4	−0.6	0.3	4.6
22	−28.5	−10.9	−18.6	−3.9	4.2	5.2	−30.0	−6.9	−0.7	2.2
23	−26.2	−1.0	−18.1	0.8	5.5	7.2	−30.5	−2.0	−0.3	4.2
24	−26.7	−1.4	−18.5	0.5	4.8	6.2	−31.4	−2.1	−0.9	3.4
25	−28.0	−1.4	−19.5	0.2	4.4	6.1	−33.0	−2.4	−1.3	3.4
26	−24.9	−0.6	−17.2	0.9	5.5	7.2	−29.4	−1.6	0.1	4.4
27	−24.8	−0.1	−17.0	1.0	5.6	7.3	−29.7	−1.2	0.1	4.5
28	−23.2	1.5	−15.7	2.4	6.4	8.2	−28.0	0.3	1.1	5.6
29	−26.2	−0.8	−18.2	0.8	5.5	7.2	−30.5	−1.9	−0.2	4.3

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Table 4 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
30	−28.8	−0.8	−20.0	0.2	4.2	6.0	−33.2	−2.1	−1.5	3.3
31	−29.0	−6.9	−19.1	−1.9	5.6	6.8	−31.4	−3.9	−0.2	3.7
32	−29.0	−0.2	−20.2	1.0	4.8	6.6	−33.8	−1.2	−1.0	4.1
33	−24.0	0.7	−16.7	1.5	5.7	7.7	−28.9	−0.9	0.4	5.0
34	−22.6	2.0	−15.3	2.8	6.8	8.6	−27.7	0.5	1.4	6.0
35	−25.4	0.2	−17.4	1.8	6.6	8.3	−29.9	−1.0	0.8	5.5
36	−27.8	1.6	−18.9	2.7	6.4	8.2	−32.7	0.5	0.4	5.7
37	−22.6	2.0	−15.4	2.8	6.9	9.0	−27.5	0.3	1.7	6.3
38	−38.3	−2.3	−26.5	−3.0	−1.8	3.0	−67.8	−8.0	−11.7	−1.3
39	−41.9	−4.2	−27.4	−3.4	−3.5	1.7	−75.0	−8.4	−13.9	−2.6
40	−38.7	−2.3	−26.8	−2.9	−1.5	3.5	−68.8	−8.4	−11.3	−0.7
41	−43.5	−3.6	−28.7	−2.8	−3.1	2.2	−77.8	−7.9	−14.0	−2.1
42	−38.3	−1.9	−26.5	−2.5	−1.1	4.0	−69.0	−8.3	−10.9	−0.2
43	−43.9	−3.3	−29.1	−2.6	−3.1	2.4	−78.6	−7.8	−14.0	−1.8
44	−38.5	−1.9	−26.8	−2.7	−1.2	3.9	−69.2	−8.4	−10.9	−0.2
45	−49.9	−15.6	−38.9	−12.6	−10.1	−2.8	−71.3	−21.4	−13.9	−6.8
46	−41.9	−25.4	−34.3	−17.6	−7.8	−4.1	−58.4	−26.9	−12.2	−8.0
47	−40.0	−11.4	−29.1	−9.3	−5.3	0.3	−55.7	−16.4	−8.7	−3.2
48	−57.8	−18.6	−45.3	−14.6	−13.1	−4.7	−79.8	−23.9	−16.4	−8.7
49	−52.6	−26.1	−41.3	−18.5	−10.0	−5.1	−68.6	−27.8	−14.4	−9.2
50	−44.9	−13.1	−32.1	−10.7	−6.7	−0.5	−62.2	−17.4	−10.1	−4.1
51	−49.5	−15.4	−38.0	−12.7	−9.4	−2.3	−69.5	−20.7	−13.0	−6.5
52	−60.4	−18.9	−47.1	−15.1	−14.1	−5.1	−82.2	−24.1	−17.3	−9.0
53	−55.7	−26.3	−43.5	−19.3	−10.9	−5.6	−72.5	−27.9	−15.7	−9.8
54	−47.0	−13.5	−33.3	−11.2	−7.1	−0.7	−64.3	−17.8	−10.7	−4.4
55	−48.6	−13.9	−37.0	−11.7	−9.2	−2.2	−67.5	−19.9	−12.5	−6.2
56	−53.1	−5.5	−32.5	−2.7	−6.4	−0.4	−63.3	−10.7	−11.7	−3.0
57	−62.7	−7.5	−39.5	−4.3	−8.9	−2.1	−72.7	−12.1	−14.2	−4.7
58	−53.3	−5.7	−33.1	−3.2	−6.7	−0.3	−63.5	−11.0	−11.7	−3.0
59	−59.1	−6.3	−38.6	−4.8	−9.8	−2.8	−72.0	−12.4	−14.8	−5.2
60	−53.2	−5.7	−33.3	−3.2	−6.6	−0.2	−63.7	−11.1	−11.6	−2.9
61	−66.2	−7.6	−42.4	−4.5	−9.6	−2.2	−77.0	−12.2	−15.1	−4.6

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Table 4 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
62	−53.2	−5.7	−33.2	−3.3	−6.6	−0.2	−63.8	−11.2	−11.6	−2.9
63	−35.2	1.6	−22.8	1.0	−1.4	3.7	−67.0	−1.1	−9.2	1.5
64	−77.8	−23.5	−55.8	−16.1	−8.2	−4.1	−67.0	−16.0	−14.1	−6.6
65	−72.3	−25.2	−52.2	−17.1	−8.4	−4.6	−61.1	−16.8	−13.8	−7.1
66	−77.7	−22.7	−56.5	−15.8	−8.1	−3.8	−67.8	−15.8	−14.0	−6.3
67	−71.8	−20.5	−52.5	−13.7	−7.3	−3.0	−62.7	−13.6	−12.6	−5.1
68	−72.4	−24.3	−52.5	−16.5	−8.0	−3.8	−61.7	−16.2	−13.4	−6.3
69	−78.6	−22.7	−57.9	−16.1	−8.8	−4.2	−69.3	−16.2	−14.8	−6.7
70	−73.0	−21.1	−53.5	−14.4	−7.9	−3.4	−64.1	−14.3	−13.0	−5.5
71	−72.7	−24.5	−53.4	−16.9	−8.6	−4.2	−62.6	−16.8	−13.9	−6.7
72	−78.1	−22.3	−57.5	−15.7	−8.3	−3.7	−69.0	−15.8	−14.3	−6.2
73	−72.7	−20.9	−53.4	−14.2	−7.7	−3.1	−64.1	−14.3	−12.8	−5.2
74	−72.8	−24.4	−53.5	−16.8	−8.5	−4.1	−62.9	−16.7	−13.8	−6.6
75	−32.4	−14.0	−0.5	5.1	3.1	6.6	−108.0	−32.4	−27.4	−10.0
76	−31.9	−11.5	−0.8	5.6	3.0	6.9	−108.2	−30.5	−27.8	−8.6
77	−32.0	−11.7	−2.1	4.2	1.7	5.5	−106.2	−29.6	−28.3	−9.6
78	−31.6	−12.9	−0.3	5.4	3.5	7.0	−107.2	−31.4	−26.9	−9.2
79	−31.9	−10.7	−0.9	6.1	3.1	7.2	−108.6	−29.6	−28.1	−7.8
80	−30.8	−10.5	−1.2	5.1	2.5	6.3	−105.0	−28.4	−27.3	−8.4
81	−31.7	−12.4	−0.6	5.7	3.2	7.0	−107.4	−30.9	−27.2	−8.8
82	−31.1	−9.8	−0.2	6.8	3.8	8.0	−107.8	−28.7	−27.3	−7.0
83	−30.9	−10.5	−0.9	5.8	3.0	6.8	−105.8	−28.8	−27.1	−7.9
84	−30.8	−11.5	0.2	6.5	4.0	7.8	−106.6	−30.0	−26.3	−7.9
85	−37.7	−14.6	−27.3	−10.4	−2.2	−1.7	−41.4	−12.5	−8.5	−5.0
86	−36.3	−14.1	−26.1	−9.7	−1.5	−0.9	−39.5	−12.1	−7.7	−4.3
87	−26.2	−8.8	−19.1	−5.9	4.5	5.1	−29.2	−8.4	−1.2	1.8
88	−35.0	−14.0	−25.1	−9.8	−1.1	−0.6	−37.7	−12.2	−7.1	−3.9
89	−37.4	−14.3	−27.6	−10.6	−2.6	−2.0	−41.4	−12.7	−8.9	−5.2
90	−36.1	−13.0	−26.0	−9.2	−1.7	−1.0	−38.8	−11.2	−7.9	−4.2
91	−37.5	−14.2	−27.7	−10.5	−2.7	−1.9	−41.5	−12.6	−9.0	−5.2
92	−35.9	−12.8	−25.8	−9.1	−1.6	−0.9	−38.6	−11.1	−7.8	−4.1
93	−35.9	−13.6	−26.0	−9.6	−1.4	−0.8	−39.4	−12.0	−7.6	−4.1

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Table 4 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
94	−35.8	−13.6	−25.9	−9.6	−1.3	−0.8	−39.4	−12.0	−7.5	−4.1
95	−35.1	−11.1	−26.3	−8.1	−1.0	−0.4	−39.6	−10.1	−7.5	−3.5
96	−35.1	−12.0	−25.1	−8.3	−0.9	−0.1	−37.9	−10.4	−7.0	−3.2
97	−35.1	−10.7	−26.2	−7.8	−0.8	−0.1	−39.7	−9.5	−7.3	−3.2
98	−23.8	−6.2	−17.6	−4.3	5.4	6.3	−27.4	−6.3	−0.1	3.1
99	−33.3	−11.4	−24.4	−8.0	−0.7	0.0	−37.2	−10.4	−6.9	−3.1
100	−34.9	−12.4	−25.3	−8.6	−0.4	0.2	−38.8	−11.0	−6.8	−3.1
101	−30.4	−11.2	−22.6	−7.8	−0.7	−0.1	−34.0	−10.9	−6.6	−3.0
102	−35.3	−12.2	−25.2	−8.4	−0.8	−0.1	−38.3	−10.7	−6.9	−3.2
103	−35.1	−10.2	−26.1	−7.5	−0.8	0.0	−39.5	−9.2	−7.4	−3.1
104	−35.1	−12.1	−24.9	−8.4	−0.5	−0.1	−38.1	−10.6	−6.7	−3.2
105	−33.6	−12.6	−24.0	−8.7	−0.3	0.4	−36.6	−11.2	−6.3	−2.8
106	−34.7	−12.4	−25.1	−8.6	−0.2	0.2	−38.6	−11.0	−6.6	−3.0
107	−49.3	−19.0	−33.4	−11.6	−6.4	−2.8	−79.2	−19.9	−17.2	−8.0
108	−44.6	−21.3	−29.5	−11.2	−5.2	−2.3	−72.2	−21.3	−14.9	−7.6
109	−50.2	−18.2	−34.5	−11.1	−6.7	−2.7	−80.7	−19.7	−17.6	−7.8
110	−46.2	−15.5	−31.6	−9.4	−5.6	−1.8	−74.3	−16.9	−15.9	−6.5
111	−45.0	−19.9	−30.5	−10.6	−5.3	−2.0	−73.9	−20.6	−15.2	−7.1
112	−50.3	−17.4	−34.5	−10.5	−6.4	−2.5	−81.4	−19.3	−17.5	−7.5
113	−46.0	−15.3	−31.4	−9.3	−5.5	−1.7	−74.3	−16.9	−15.6	−6.4
114	−45.4	−19.2	−30.9	−10.3	−5.2	−1.7	−74.9	−20.1	−15.4	−6.7
115	−50.0	−17.1	−34.3	−10.3	−6.2	−2.3	−81.2	−19.1	−17.3	−7.3
116	−46.3	−15.6	−31.7	−9.6	−5.6	−1.9	−74.8	−17.4	−15.8	−6.6
117	−45.5	−19.0	−31.0	−10.3	−5.3	−1.6	−75.1	−20.1	−15.4	−6.6
118	−48.4	−25.8	−40.1	−20.3	−11.5	−7.4	−66.6	−28.3	−16.5	−11.6
119	−41.1	−17.9	−32.8	−15.4	−9.3	−4.7	−57.9	−22.5	−12.8	−8.5
120	−47.1	−26.7	−39.6	−20.4	−10.8	−6.7	−64.9	−28.6	−15.6	−10.9
121	−43.6	−18.7	−33.8	−15.9	−9.5	−5.1	−60.2	−22.5	−13.5	−9.0
122	−46.8	−22.9	−39.0	−18.1	−10.4	−5.6	−66.4	−25.7	−15.2	−9.8
123	−42.9	−17.4	−34.4	−14.8	−9.0	−4.2	−59.8	−22.3	−12.4	−7.9
124	−49.6	−26.0	−41.4	−21.1	−12.0	−7.7	−70.1	−28.4	−16.9	−11.8
125	−44.7	−17.1	−35.2	−15.1	−9.7	−5.0	−61.2	−21.6	−13.6	−8.7

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Table 4 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
126	−43.2	−17.5	−34.0	−15.3	−9.4	−4.7	−59.7	−21.8	−13.1	−8.5
127	−50.3	−24.1	−40.8	−19.4	−11.3	−6.6	−69.9	−26.8	−16.4	−10.9
128	−67.1	−21.0	−42.3	−13.6	−11.7	−7.1	−73.9	−21.3	−18.0	−10.3
129	−63.7	−21.7	−40.1	−13.8	−11.8	−7.4	−69.4	−21.3	−17.6	−10.6
130	−65.9	−19.8	−42.1	−13.0	−11.4	−6.3	−73.3	−20.4	−17.5	−9.5
131	−62.9	−18.5	−40.5	−11.8	−10.6	−5.8	−69.8	−18.8	−16.2	−8.5
132	−63.3	−21.0	−40.2	−13.5	−11.5	−6.8	−69.5	−20.8	−17.2	−10.0
133	−68.2	−20.4	−44.1	−13.7	−12.4	−7.0	−76.1	−21.2	−18.8	−10.2
134	−63.0	−18.8	−40.8	−12.1	−11.1	−6.1	−70.1	−19.2	−16.5	−8.8
135	−63.7	−21.0	−41.0	−13.6	−12.0	−6.9	−70.4	−21.0	−17.8	−10.1
136	−67.8	−20.0	−43.7	−13.4	−12.1	−6.7	−75.8	−20.9	−18.3	−9.9
137	−63.2	−18.8	−41.0	−12.2	−11.1	−6.0	−70.5	−19.4	−16.6	−8.7
138	−63.7	−20.7	−41.1	−13.5	−12.0	−6.7	−70.7	−20.9	−17.7	−9.9
139	−41.2	−14.4	−26.8	−8.4	−5.0	−1.6	−68.7	−13.8	−13.0	−4.8
140	−42.4	−13.0	−28.2	−7.4	−5.0	−1.2	−70.8	−13.3	−13.4	−4.3
141	−38.4	−11.2	−25.2	−6.5	−4.3	−0.9	−64.8	−11.5	−11.8	−3.7
142	−64.6	−29.4	−50.0	−19.1	−2.3	−0.6	−66.8	−25.8	−15.5	−7.6
143	−60.2	−28.4	−46.8	−18.0	−1.3	0.5	−61.1	−23.5	−14.4	−6.8
144	−60.1	−29.7	−47.3	−18.8	−1.7	0.1	−61.1	−24.4	−14.6	−7.2
145	−65.8	−32.4	−50.9	−21.6	−4.2	−2.5	−67.6	−28.6	−16.5	−9.0
146	−61.5	−31.2	−47.8	−20.6	−3.1	−1.6	−62.3	−26.4	−15.5	−8.5
147	−63.0	−32.8	−48.5	−21.2	−3.3	−1.6	−63.1	−27.1	−15.5	−8.5
148	−22.9	−12.0	5.7	9.8	7.1	9.8	−81.5	−32.6	−20.8	−8.1
149	−34.4	−13.2	−5.2	1.3	−4.6	−0.6	−112.4	−41.3	−35.6	−15.9
150	−51.0	−20.2	−39.5	−11.4	4.9	7.4	−56.1	−16.2	−7.4	−0.1
151	−45.2	−7.4	−43.1	−5.9	0.4	5.2	−57.9	−9.8	−11.0	−0.5
152	−31.7	−12.8	−21.0	−4.3	−2.7	0.5	−52.7	−15.1	−9.3	−3.7
153	−29.8	−4.7	−24.5	−4.6	−5.9	−1.6	−55.8	−15.1	−12.4	−5.4
154	−36.3	−17.2	−19.0	−3.8	1.4	4.1	−55.1	−16.3	−8.3	−1.9
155	−39.4	−14.4	−27.5	−7.4	−4.1	−0.6	−59.1	−16.9	−10.9	−4.8
156	−31.3	−5.6	−19.6	−1.5	−1.7	2.2	−57.6	−9.9	−10.1	−1.9
157	−39.3	−11.6	−29.5	−8.3	−4.0	0.0	−60.2	−16.6	−11.1	−4.7

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Table 4 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
158	−22.7	−11.8	5.6	9.6	7.6	10.4	−81.4	−32.3	−20.4	−7.6
159	−23.0	−12.0	5.2	9.4	7.3	10.0	−81.9	−32.8	−20.8	−8.0
160	−50.6	−19.9	−39.4	−11.3	5.4	7.9	−55.9	−16.2	−7.0	0.2
161	−42.0	−3.4	−40.5	−2.4	3.7	8.3	−53.3	−4.5	−8.1	2.8
162	−32.5	−15.9	−20.5	−4.5	−1.0	1.8	−49.1	−18.5	−8.2	−3.6
163	−32.3	−5.5	−24.7	−3.5	−4.2	0.7	−58.6	−12.6	−11.0	−3.6
164	−37.0	−17.6	−21.0	−4.7	1.1	3.3	−52.3	−16.7	−8.3	−2.5
165	−35.8	−18.8	−22.3	−6.7	−2.4	0.3	−52.5	−20.1	−9.9	−5.2
166	−38.8	−8.3	−23.9	−3.7	−1.3	2.9	−66.6	−12.0	−11.3	−1.9
167	−45.1	−18.0	−31.1	−9.9	−5.0	−1.4	−65.2	−22.1	−12.5	−6.4
168	−22.7	−11.7	5.7	9.8	8.0	10.8	−81.5	−32.1	−20.0	−7.2
169	−23.0	−11.7	5.4	9.7	7.8	10.5	−82.5	−32.3	−20.4	−7.5
170	−51.4	−21.2	−40.0	−12.4	3.5	6.2	−56.0	−17.2	−8.6	−1.4
171	−58.6	−19.6	−50.2	−13.4	0.0	3.6	−68.6	−18.9	−13.5	−3.4
172	−34.7	−15.8	−21.1	−3.7	−2.8	0.8	−57.3	−18.6	−10.3	−4.5
173	−39.8	−9.9	−29.7	−5.7	−5.8	−1.1	−67.9	−14.8	−13.3	−5.1
174	−35.7	−19.2	−22.3	−6.7	−1.9	0.8	−52.1	−19.9	−9.1	−4.6
175	−45.7	−12.4	−27.8	−5.0	−1.9	2.4	−73.7	−14.3	−12.5	−2.5
176	−46.1	−16.5	−30.5	−9.5	−5.6	−0.9	−70.6	−16.8	−13.8	−5.0
177	−22.1	−11.2	6.1	10.2	8.5	11.3	−80.6	−31.6	−19.5	−6.6
178	−33.3	−6.6	−4.0	3.9	−2.0	2.6	−116.1	−29.1	−33.7	−10.2
179	−51.1	−20.9	−39.7	−12.1	3.9	6.6	−55.8	−17.0	−8.2	−1.0
180	−51.5	−20.7	−40.4	−12.2	4.7	7.3	−57.0	−17.2	−7.8	−0.5
181	−41.0	−15.1	−27.8	−5.7	−5.3	−0.7	−67.4	−18.7	−12.8	−5.5
182	−41.2	−14.2	−28.5	−5.6	−5.5	−0.7	−68.2	−18.0	−12.9	−5.2
183	−35.7	−16.4	−19.8	−3.6	2.3	4.5	−51.0	−15.8	−7.1	−1.3
184	−35.1	−18.7	−21.7	−6.2	−1.4	1.3	−51.3	−19.4	−8.6	−4.1
185	−43.0	−13.7	−25.6	−4.2	−0.8	3.2	−70.1	−14.8	−11.1	−1.9
186	−43.4	−19.0	−27.9	−8.5	−4.0	0.0	−65.6	−18.1	−12.1	−4.2
187	−32.4	−12.1	0.0	6.4	2.7	6.6	−107.1	−35.0	−29.4	−10.2
188	−63.5	−21.4	−53.6	−15.6	−1.0	2.6	−74.3	−22.8	−15.0	−5.0
189	−48.5	−20.2	−33.9	−9.4	−9.3	−4.8	−76.6	−25.3	−17.9	−10.2

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Table 4 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
190	−53.6	−22.6	−34.7	−11.8	−7.3	−3.6	−82.4	−25.2	−18.9	−9.5
191	−52.6	−26.6	−35.9	−14.9	−9.6	−5.9	−76.9	−28.0	−19.1	−11.1
192	−33.3	−9.8	0.1	7.4	3.2	7.5	−111.4	−31.3	−29.7	−8.4
193	−65.2	−21.7	−55.9	−15.8	−1.6	2.3	−76.8	−22.5	−15.8	−5.1
194	−51.2	−21.1	−36.2	−10.2	−10.8	−5.7	−80.6	−26.3	−19.2	−11.0
195	−56.4	−23.4	−35.9	−12.2	−8.1	−4.1	−86.5	−25.9	−19.8	−9.9
196	−56.1	−28.4	−38.0	−15.9	−11.1	−7.1	−81.7	−29.1	−20.5	−12.1
197	−31.4	−7.3	0.4	7.5	4.4	8.6	−111.6	−23.3	−27.5	−5.8
198	−60.6	−11.6	−54.8	−11.3	−0.2	3.7	−72.3	−12.4	−13.7	−2.3
199	−46.1	−12.6	−36.4	−8.5	−8.0	−2.9	−76.3	−17.0	−16.1	−7.3
200	−50.7	−12.8	−35.1	−8.7	−6.2	−1.8	−82.9	−15.0	−17.5	−6.7
201	−57.1	−18.8	−42.8	−13.7	−9.6	−5.0	−79.8	−21.3	−18.0	−9.7
202	−29.3	−11.6	0.7	6.9	3.0	6.6	−95.8	−35.5	−28.3	−10.6
203	−64.0	−24.9	−53.6	−17.7	−1.7	1.6	−72.1	−23.3	−15.7	−6.3
204	−43.8	−21.0	−30.3	−9.7	−7.3	−3.6	−65.6	−25.5	−15.7	−9.4
205	−48.2	−23.4	−30.0	−10.7	−5.3	−2.3	−72.0	−24.7	−16.4	−8.5
206	−49.4	−29.0	−32.6	−15.2	−8.7	−5.7	−70.0	−28.9	−17.6	−11.1
207	−31.5	−10.1	−0.4	5.8	2.4	6.2	−106.3	−26.1	−27.9	−8.8
208	−56.0	−12.2	−49.9	−11.6	−0.8	2.7	−64.7	−11.7	−13.3	−3.3
209	−43.9	−16.1	−32.6	−9.5	−8.8	−4.7	−71.1	−18.9	−16.1	−8.9
210	−46.8	−16.2	−31.4	−9.7	−6.0	−2.5	−74.8	−16.8	−16.0	−7.2
211	−41.6	−16.0	−30.1	−11.0	−7.3	−3.7	−63.4	−15.5	−15.0	−7.3
212	−28.8	−13.3	0.6	6.1	2.8	5.9	−93.9	−36.9	−27.9	−12.2
213	−60.0	−25.3	−49.6	−16.8	0.3	3.4	−67.4	−23.0	−13.4	−4.9
214	−45.7	−21.5	−29.6	−8.8	−7.4	−3.4	−70.9	−24.4	−15.8	−9.0
215	−45.2	−23.2	−25.8	−8.6	−1.9	1.0	−68.1	−23.3	−12.4	−5.5
216	−49.8	−27.1	−32.6	−13.1	−7.5	−4.5	−69.4	−29.0	−16.0	−10.6
217	−30.6	−12.6	0.9	6.9	2.9	6.4	−101.5	−34.7	−28.6	−11.3
218	−64.9	−25.6	−54.4	−17.6	−1.4	2.1	−73.6	−23.5	−15.7	−6.1
219	−48.1	−21.2	−32.5	−9.3	−9.0	−4.6	−75.1	−24.4	−17.6	−10.3
220	−49.7	−22.8	−31.7	−10.0	−5.3	−2.2	−72.9	−24.8	−16.3	−8.6
221	−55.8	−26.9	−37.1	−13.5	−7.6	−3.9	−75.0	−28.3	−16.4	−10.0

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Table 4 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
222	−31.0	−4.7	−0.2	7.0	3.9	8.0	−108.9	−16.6	−28.0	−5.7
223	−63.5	−24.4	−53.6	−16.9	−0.5	3.1	−72.7	−23.0	−14.7	−5.1
224	−47.1	−15.7	−36.6	−11.3	−9.3	−4.8	−75.9	−18.3	−17.4	−9.0
225	−44.5	−20.8	−27.4	−8.2	−2.2	0.6	−65.8	−22.9	−13.1	−5.9
226	−52.1	−27.4	−35.0	−14.5	−8.6	−4.9	−76.2	−27.4	−18.2	−10.3
227	−30.2	−14.4	0.5	5.6	1.8	4.8	−99.3	−36.2	−28.8	−13.3
228	−55.8	−26.2	−46.1	−18.0	−1.2	1.4	−61.3	−22.9	−13.4	−6.3
229	−43.6	−21.4	−29.8	−10.3	−7.6	−4.6	−65.3	−24.4	−16.3	−10.0
230	−38.7	−18.5	−24.5	−7.8	−2.3	−0.3	−52.8	−18.9	−11.6	−5.5
231	−41.5	−26.1	−23.0	−10.5	−4.7	−1.9	−57.9	−23.7	−12.5	−7.2
232	−29.6	−13.2	1.1	6.3	2.8	5.9	−99.8	−34.7	−27.8	−11.9
233	−61.3	−23.7	−50.8	−16.0	0.0	3.3	−69.2	−21.3	−13.3	−4.5
234	−45.1	−19.4	−29.9	−7.5	−7.5	−3.5	−72.0	−22.1	−15.9	−8.9
235	−47.8	−21.9	−30.7	−9.7	−2.8	−0.2	−70.1	−22.9	−13.6	−6.2
236	−44.9	−24.3	−29.7	−11.3	−6.7	−3.7	−62.2	−26.8	−14.5	−9.7
MAXD	−78.6	−32.8	−57.9	−21.6	−14.1	11.3	−116.1	−41.3	−35.6	−15.9
MD	−44.3	−14.4	−27.8	−6.5	−2.7	0.9	−67.9	−18.3	−14.4	−5.3
MAD	44.3	14.5	28.3	9.2	5.2	4.1	67.9	18.3	14.4	6.1

Table 5: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the BP86 functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−16.3	28.4	−3.7	28.4	27.0	32.3	−12.1	28.6	24.2	31.0
2	−20.9	29.3	−6.1	29.5	27.9	33.8	−15.2	30.7	25.0	32.4
3	−18.4	26.3	−5.6	26.5	26.0	31.5	−14.0	27.0	23.3	30.1
4	−21.4	30.5	−6.3	30.7	29.2	35.2	−15.7	31.9	26.1	33.8
5	−19.7	28.9	−6.1	28.8	28.0	33.8	−15.1	29.5	24.9	32.3
6	−21.3	31.2	−6.3	31.3	29.7	35.9	−15.9	32.4	26.6	34.4
7	−19.3	29.2	−5.8	29.1	28.5	34.2	−14.9	29.7	25.4	32.6

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Table 5 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
8	−13.4	6.4	10.5	16.2	9.5	13.8	−84.3	−13.1	−15.1	2.9
9	−12.5	8.7	11.9	18.0	11.4	15.8	−85.6	−9.0	−13.8	5.3
10	−21.8	−7.5	7.1	11.6	6.7	10.1	−84.7	−24.8	−18.1	−3.6
11	−19.3	−4.3	8.3	13.0	8.6	11.9	−83.9	−20.7	−16.3	−1.4
12	−12.6	7.4	11.1	17.0	10.5	14.9	−84.1	−12.2	−14.2	4.0
13	−10.6	10.8	13.8	20.0	13.3	17.9	−84.0	−7.2	−11.9	7.4
14	−21.3	−6.8	7.5	12.1	7.2	10.6	−84.4	−24.3	−17.6	−3.0
15	−17.1	0.2	10.7	15.8	11.2	14.9	−84.1	−14.3	−14.1	2.4
16	−9.7	12.2	14.1	20.4	13.9	18.5	−83.1	−7.0	−11.4	8.1
17	−10.0	11.5	14.4	20.8	14.1	18.6	−83.7	−6.6	−11.3	8.2
18	−20.4	−5.5	8.4	13.4	8.2	11.7	−83.9	−22.9	−16.8	−1.5
19	−16.3	1.8	11.5	16.9	12.0	15.8	−84.0	−12.4	−13.4	3.8
20	−9.2	12.8	14.6	21.0	14.5	19.2	−83.0	−6.5	−10.8	8.7
21	12.3	31.5	17.0	31.6	34.1	36.1	8.9	31.5	31.2	34.5
22	−6.3	7.6	1.6	13.5	19.0	20.2	−6.1	12.1	16.3	18.5
23	14.4	33.9	19.1	34.3	37.2	39.2	11.4	33.7	33.8	37.3
24	12.0	31.7	17.0	32.2	34.7	36.4	8.7	31.6	31.4	34.7
25	11.5	32.3	16.7	32.5	35.0	37.0	7.9	32.0	31.7	35.3
26	11.6	30.6	16.4	30.9	33.7	35.6	8.4	30.3	30.6	33.9
27	12.2	31.4	16.8	31.3	34.2	36.2	8.5	31.0	31.1	34.5
28	14.6	33.9	19.0	33.6	36.0	38.1	11.3	33.6	33.1	36.6
29	14.9	34.7	19.6	35.0	37.9	39.9	11.9	34.4	34.5	38.0
30	14.5	36.3	19.8	36.1	38.4	40.5	11.4	35.8	35.1	38.9
31	2.2	19.6	9.5	23.5	28.7	30.1	1.6	23.2	25.1	28.1
32	13.6	36.1	19.0	36.0	38.2	40.3	10.2	35.9	34.9	38.8
33	15.9	35.2	20.1	34.8	37.3	39.6	12.4	34.3	34.4	38.0
34	15.6	34.9	19.8	34.5	36.9	38.9	12.0	34.2	33.8	37.4
35	16.4	36.4	21.1	36.7	39.6	41.6	13.2	35.9	36.2	39.8
36	16.2	39.3	21.6	39.0	41.2	43.3	12.7	38.9	37.7	41.8
37	17.6	36.8	21.7	36.4	38.9	41.3	14.0	35.9	36.0	39.6
38	6.4	35.9	13.8	33.9	34.6	39.6	−18.7	31.0	28.3	36.6
39	6.1	36.9	15.9	36.4	35.5	40.8	−22.0	33.5	28.8	37.8

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Table 5 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
40	6.5	36.4	14.2	34.5	35.5	40.8	−19.2	31.2	29.2	37.7
41	6.5	39.2	16.7	38.8	37.7	43.2	−22.5	35.8	30.7	40.2
42	7.3	37.2	14.8	35.3	36.3	41.7	−19.0	31.6	30.0	38.6
43	7.4	40.7	17.5	40.1	38.9	44.6	−22.0	37.1	31.9	41.6
44	7.2	37.3	14.6	35.2	36.4	41.7	−19.1	31.6	30.1	38.6
45	17.6	45.2	23.9	46.7	46.9	54.7	0.9	41.3	45.9	51.7
46	−9.3	4.6	−3.7	11.4	19.2	23.1	−21.8	3.6	16.9	20.2
47	10.9	33.5	17.7	34.2	35.8	41.8	−1.3	29.7	34.9	39.2
48	18.8	50.6	26.2	52.7	51.8	60.8	1.8	47.1	51.3	57.6
49	−6.3	15.8	2.0	22.1	28.3	33.5	−17.9	15.0	26.1	30.3
50	9.7	34.8	18.2	36.0	37.6	44.2	−3.8	31.7	36.7	41.4
51	17.4	44.7	24.4	46.0	47.2	54.7	1.8	41.0	46.3	51.5
52	19.8	53.5	27.7	55.5	54.1	63.6	3.0	50.1	53.7	60.5
53	−4.5	19.8	4.5	25.7	31.7	37.4	−16.6	19.3	29.4	34.0
54	9.8	36.3	19.1	37.4	39.1	45.9	−3.6	33.3	38.1	43.1
55	19.0	46.8	26.1	47.6	48.0	55.6	4.3	42.5	47.4	52.5
56	−6.6	33.1	9.3	34.2	28.8	34.7	−14.2	28.9	26.1	33.0
57	−10.1	36.1	8.0	37.4	30.9	37.7	−17.3	32.5	28.3	35.9
58	−6.7	33.1	9.1	34.0	28.8	35.0	−14.3	28.8	26.2	33.2
59	−6.7	37.4	9.0	37.1	30.4	37.3	−16.6	32.1	27.8	35.5
60	−6.5	33.2	9.0	34.0	29.0	35.3	−14.4	28.7	26.4	33.4
61	−9.7	39.5	9.1	40.7	33.9	41.2	−17.4	35.9	31.1	39.4
62	−6.3	33.3	9.2	34.1	29.2	35.5	−14.3	28.8	26.6	33.6
63	18.3	48.2	26.3	46.6	43.6	48.9	−8.0	46.7	39.2	47.6
64	−40.7	5.2	−22.4	11.2	17.0	21.0	−30.7	12.6	13.1	19.1
65	−40.9	−1.1	−23.9	5.8	12.5	16.3	−30.5	7.2	9.0	14.4
66	−39.5	7.0	−21.7	12.6	18.4	22.6	−30.2	13.9	14.4	20.7
67	−37.6	5.6	−21.6	11.0	15.6	19.8	−29.0	12.4	12.1	18.1
68	−40.2	0.5	−23.3	7.2	13.7	17.8	−30.2	8.5	10.2	16.0
69	−39.3	7.9	−22.0	13.3	18.7	23.1	−30.7	14.5	14.6	21.2
70	−38.4	5.4	−22.1	10.8	15.5	19.9	−29.9	12.2	12.1	18.2
71	−39.8	1.0	−23.3	7.5	14.0	18.2	−30.3	8.7	10.5	16.3

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Table 5 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
72	−38.6	8.6	−21.4	13.9	19.4	23.8	−30.2	15.1	15.4	21.9
73	−37.6	6.0	−21.6	11.4	16.2	20.5	−29.5	12.6	12.8	18.9
74	−39.7	1.3	−23.2	7.8	14.3	18.5	−30.4	8.9	10.8	16.6
75	−21.9	−6.9	7.2	11.6	7.6	10.9	−90.1	−25.0	−17.6	−3.4
76	−18.4	−1.9	9.6	14.7	10.5	14.1	−87.1	−20.4	−14.8	0.7
77	−19.7	−3.2	7.1	12.1	8.1	11.6	−86.2	−20.5	−16.6	−1.4
78	−20.4	−5.2	8.2	12.7	8.9	12.1	−88.5	−23.4	−16.2	−1.9
79	−17.8	−0.5	10.1	15.6	11.1	14.9	−86.8	−19.0	−14.4	2.0
80	−18.1	−1.6	8.5	13.5	9.5	13.0	−84.6	−18.9	−15.0	0.3
81	−20.0	−4.3	8.4	13.3	9.2	12.7	−88.2	−22.5	−15.9	−1.0
82	−16.9	0.4	10.9	16.4	12.0	15.8	−85.9	−18.0	−13.5	2.9
83	−18.0	−1.4	9.0	14.3	10.1	13.7	−85.3	−19.3	−14.6	0.9
84	−19.0	−3.3	9.3	14.2	10.1	13.6	−87.3	−21.5	−14.9	0.0
85	−8.4	9.6	−0.5	12.9	19.3	19.9	−10.2	12.5	15.0	17.6
86	−4.3	13.1	3.2	16.2	22.4	23.1	−5.6	15.9	18.1	20.8
87	1.8	15.0	6.8	17.2	26.0	26.7	0.3	16.2	22.1	24.4
88	−4.3	12.0	3.1	15.3	21.9	22.5	−5.2	14.8	17.7	20.2
89	−7.4	10.7	0.1	13.6	19.8	20.5	−9.5	13.1	15.5	18.3
90	−3.3	14.7	4.1	17.4	23.0	23.7	−4.2	17.3	18.8	21.5
91	−7.5	10.7	0.0	13.6	19.6	20.5	−9.6	13.1	15.4	18.3
92	−3.1	14.9	4.2	17.5	23.1	23.9	−4.0	17.5	18.9	21.7
93	−3.3	14.1	3.9	17.0	23.3	23.9	−4.9	16.7	19.0	21.7
94	−3.2	14.1	4.1	17.0	23.4	24.0	−4.8	16.7	19.2	21.7
95	−3.3	15.6	3.3	17.7	23.1	23.8	−5.8	17.5	18.6	21.6
96	−2.2	15.9	5.2	18.6	24.1	24.9	−3.1	18.5	19.9	22.8
97	−3.0	16.1	3.5	18.2	23.4	24.2	−5.6	18.1	19.0	22.1
98	4.3	17.8	8.7	19.2	27.4	28.3	2.4	18.7	23.5	26.0
99	−1.1	16.1	5.5	18.5	24.0	24.9	−3.1	18.0	19.8	22.7
100	−1.9	15.8	5.2	18.5	24.8	25.5	−3.8	18.1	20.3	23.2
101	2.4	17.4	8.0	19.8	25.1	25.8	0.4	18.7	21.0	23.7
102	−2.2	15.8	5.3	18.6	24.3	25.1	−3.3	18.3	20.1	22.9
103	−2.0	17.6	4.6	19.5	24.4	25.3	−4.3	19.6	19.9	23.2

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Table 5 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
104	−2.0	15.9	5.5	18.6	24.6	25.1	−3.2	18.3	20.3	23.0
105	−1.4	15.0	5.8	18.1	24.6	25.3	−2.7	17.3	20.3	23.0
106	−1.6	15.9	5.5	18.6	25.1	25.6	−3.5	18.1	20.7	23.3
107	−11.6	13.2	0.7	19.4	23.2	26.8	−36.4	13.0	15.6	22.9
108	−16.7	2.4	−4.3	11.4	15.9	18.8	−39.9	2.6	9.0	14.9
109	−10.3	16.2	2.0	22.1	25.1	29.2	−35.6	15.4	17.5	25.3
110	−10.0	15.4	1.2	20.2	22.7	26.5	−33.2	14.7	15.5	22.9
111	−14.1	6.6	−2.3	14.8	18.6	22.0	−38.5	6.2	11.7	18.1
112	−8.6	18.6	3.7	24.3	27.0	31.0	−34.5	17.5	19.3	27.2
113	−9.3	15.9	1.9	20.7	23.3	27.1	−32.7	15.2	16.2	23.5
114	−13.1	8.6	−1.3	16.4	20.1	23.7	−37.9	8.0	12.9	19.8
115	−8.1	19.1	4.1	24.7	27.5	31.5	−34.1	17.9	19.7	27.7
116	−8.9	16.4	2.3	21.2	24.0	27.6	−32.5	15.3	16.8	24.1
117	−12.8	9.0	−1.1	16.8	20.3	24.0	−37.8	8.3	13.2	20.2
118	−1.2	17.4	4.4	21.7	28.1	32.5	−14.8	16.2	25.3	29.2
119	1.8	20.3	7.4	21.9	25.7	30.6	−11.4	16.9	24.2	27.6
120	−4.2	12.5	0.9	17.7	24.9	29.2	−17.5	11.7	22.1	25.8
121	0.3	19.9	7.0	21.8	25.9	30.6	−12.6	17.5	24.1	27.7
122	2.5	22.1	7.6	25.7	31.1	36.2	−12.4	20.7	28.5	32.8
123	2.9	23.2	8.9	25.0	28.4	33.5	−10.4	19.5	26.9	30.5
124	−0.5	18.5	4.8	22.3	29.2	33.8	−16.1	17.6	26.4	30.4
125	3.7	25.4	10.0	26.5	29.6	34.5	−8.8	22.4	27.7	31.5
126	1.9	22.3	8.2	23.6	27.2	32.2	−10.8	19.3	25.6	29.2
127	2.5	23.7	8.8	27.3	33.1	38.1	−12.3	22.5	30.3	34.6
128	−26.7	11.7	−5.7	17.8	17.7	22.3	−30.8	12.2	14.0	20.0
129	−28.4	6.6	−8.1	13.4	13.6	17.8	−31.6	7.7	10.1	15.7
130	−25.3	12.9	−5.1	18.8	18.5	23.5	−29.9	13.3	14.8	21.2
131	−24.9	12.0	−6.0	17.5	16.9	21.6	−29.1	12.5	13.5	19.6
132	−27.1	8.2	−7.1	14.7	14.9	19.4	−30.7	9.1	11.5	17.2
133	−24.9	14.9	−4.4	20.5	19.9	25.2	−29.9	15.0	16.0	22.8
134	−24.9	12.0	−6.0	17.5	16.8	21.6	−29.1	12.5	13.5	19.6
135	−26.5	9.1	−6.9	15.5	15.3	20.3	−30.6	9.8	12.0	18.1

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Table 5 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
136	−24.3	15.5	−3.8	21.0	20.5	25.7	−29.5	15.4	16.7	23.4
137	−24.2	12.7	−5.4	18.2	17.5	22.4	−28.7	13.0	14.3	20.4
138	−26.0	10.0	−6.5	16.2	15.9	21.0	−30.3	10.5	12.6	18.8
139	−2.4	19.3	8.6	24.4	26.6	30.0	−24.8	20.6	21.4	27.8
140	0.5	24.5	11.4	29.3	30.4	34.3	−22.8	25.1	25.0	32.1
141	−0.4	21.7	9.5	25.6	26.6	30.0	−21.8	22.3	21.6	28.0
142	−41.8	−12.5	−29.1	−3.3	11.2	12.9	−42.6	−8.5	0.9	7.3
143	−39.4	−12.8	−27.6	−3.6	10.6	12.4	−38.8	−7.5	0.3	6.5
144	−38.0	−12.7	−27.2	−3.4	10.9	12.8	−37.9	−7.4	1.0	7.0
145	−42.6	−14.9	−29.4	−5.1	9.5	11.2	−42.8	−10.5	0.1	6.1
146	−40.3	−15.2	−28.1	−5.4	9.0	10.6	−39.4	−9.6	−0.7	5.0
147	−40.6	−15.6	−28.1	−5.3	9.2	11.0	−39.3	−9.5	0.0	5.7
148	−18.5	−9.6	7.2	10.4	5.8	8.3	−71.7	−30.0	−17.0	−6.7
149	−24.6	−7.4	0.6	5.8	−0.8	3.0	−95.5	−34.6	−25.9	−9.9
150	−37.4	−11.5	−27.1	−3.6	9.9	12.4	−40.4	−7.3	1.1	6.8
151	−10.4	21.0	−10.0	21.3	25.3	30.3	−20.8	19.1	17.9	26.3
152	−11.0	4.2	−1.9	12.3	11.4	14.8	−28.5	2.5	7.9	12.2
153	5.1	25.3	7.9	24.7	21.9	26.5	−17.1	16.3	18.3	23.9
154	−17.4	−1.7	−3.0	10.2	13.7	16.5	−33.2	−0.8	7.0	12.1
155	−7.6	12.7	1.6	18.7	19.9	23.7	−23.4	11.2	15.8	20.6
156	1.0	22.3	9.7	25.2	23.9	27.9	−21.5	18.6	18.5	25.1
157	−1.9	20.3	4.6	22.3	24.7	29.0	−19.4	16.2	20.5	25.5
158	−18.2	−9.3	7.3	10.5	6.5	9.1	−71.5	−29.6	−16.4	−6.0
159	−18.4	−9.4	7.0	10.3	6.3	8.8	−71.9	−30.0	−16.8	−6.4
160	−36.8	−11.1	−26.8	−3.3	10.7	13.1	−40.1	−7.1	1.7	7.4
161	−6.4	25.6	−6.5	25.4	29.1	33.7	−14.9	25.4	21.4	30.0
162	−14.6	−1.2	−4.3	9.5	10.2	13.1	−28.2	−3.2	6.0	9.6
163	5.0	26.5	9.8	27.6	25.0	30.2	−17.5	20.6	21.8	27.6
164	−20.2	−4.2	−6.8	7.3	11.6	13.8	−32.8	−3.2	5.0	9.6
165	−14.3	−0.6	−3.3	10.3	12.1	14.9	−27.7	−1.0	7.3	11.0
166	−2.8	22.1	8.3	25.5	26.8	31.2	−26.5	19.0	20.3	27.8
167	−11.3	10.4	−0.4	17.5	20.1	23.9	−27.8	7.4	15.5	20.4

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Table 5 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
168	−18.0	−9.0	7.5	10.8	7.0	9.6	−71.4	−29.3	−15.9	−5.5
169	−18.1	−8.9	7.5	10.9	7.0	9.6	−72.1	−29.4	−16.1	−5.6
170	−37.7	−12.2	−27.4	−4.3	8.9	11.5	−40.2	−7.9	0.1	5.8
171	−35.6	−3.3	−28.5	2.1	13.0	16.6	−43.1	−2.0	3.4	11.4
172	−9.9	5.3	1.7	16.6	14.4	18.1	−28.8	3.3	10.4	14.8
173	−1.6	22.4	5.9	26.0	23.9	28.7	−24.7	18.9	19.8	26.2
174	−15.5	−2.1	−4.4	9.2	11.6	14.3	−28.5	−2.0	6.9	10.5
175	−10.3	16.8	3.5	22.8	24.9	29.3	−33.9	15.3	17.8	25.7
176	−7.7	16.3	4.1	22.1	24.1	29.0	−27.5	17.0	19.3	26.2
177	−17.5	−8.6	7.9	11.2	7.5	10.1	−70.6	−28.9	−15.4	−5.0
178	−18.2	3.5	6.7	12.9	6.6	11.1	−92.7	−18.0	−18.8	0.3
179	−37.4	−12.0	−27.1	−4.0	9.2	11.8	−40.0	−7.6	0.4	6.1
180	−37.5	−11.7	−27.5	−4.0	10.2	12.7	−40.9	−7.8	1.1	6.9
181	−7.7	13.0	3.0	21.7	19.4	24.1	−29.6	10.3	15.5	21.3
182	−6.3	15.4	4.0	23.4	20.7	25.7	−28.7	12.6	17.1	23.0
183	−18.8	−3.0	−5.6	8.5	12.8	15.0	−31.4	−2.3	6.2	10.8
184	−15.0	−1.7	−3.9	9.6	12.0	14.7	−27.9	−1.6	7.3	10.9
185	−10.8	13.2	3.0	21.3	23.4	27.5	−33.6	12.4	16.4	23.8
186	−11.8	8.1	0.7	17.4	19.8	23.9	−29.5	9.9	14.7	21.0
187	−19.4	−2.8	9.1	14.1	8.8	12.4	−86.1	−24.5	−17.1	−1.6
188	−35.0	0.2	−26.8	5.1	16.7	20.3	−43.0	0.0	6.6	14.5
189	−9.5	13.4	2.0	22.9	20.1	24.7	−32.8	9.6	15.2	21.2
190	−15.1	10.6	−0.4	19.5	22.5	26.2	−39.2	8.7	14.3	21.8
191	−15.4	6.0	−2.4	16.1	19.0	22.8	−34.9	5.8	12.6	19.0
192	−17.9	1.2	11.2	17.0	11.4	15.4	−87.7	−19.0	−15.1	2.2
193	−36.0	0.3	−28.1	5.3	16.7	20.5	−44.7	0.4	6.4	14.9
194	−9.1	15.2	2.7	24.8	21.3	26.5	−33.6	11.2	16.7	23.0
195	−15.9	11.4	0.3	20.8	23.2	27.3	−41.2	9.5	15.0	23.0
196	−16.4	6.4	−2.0	17.3	19.6	23.7	−36.9	7.0	13.4	20.1
197	−15.0	4.5	13.0	18.6	14.0	18.0	−86.8	−10.8	−11.9	5.6
198	−27.0	13.7	−22.5	13.6	22.7	26.5	−35.5	14.1	13.1	22.1
199	−0.6	26.3	6.2	29.6	27.7	33.0	−25.5	23.1	23.4	30.2

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Table 5 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
200	−3.6	27.8	7.6	30.4	31.6	36.0	−30.4	26.4	23.9	32.6
201	−5.9	25.2	4.3	28.8	30.7	35.5	−24.3	23.9	25.5	32.0
202	−18.9	−4.4	7.7	12.6	7.3	10.7	−78.3	−26.8	−18.1	−3.9
203	−41.0	−8.2	−31.7	−1.6	11.4	14.6	−46.3	−5.6	1.0	8.5
204	−15.0	3.5	−3.6	14.0	13.4	17.2	−32.9	0.2	8.2	13.2
205	−18.9	1.7	−3.8	12.9	16.5	19.6	−38.5	1.1	8.5	14.8
206	−20.5	−3.7	−6.5	8.7	12.6	15.7	−36.7	−2.4	6.6	11.8
207	−19.2	−1.9	8.6	13.5	8.5	12.0	−86.1	−17.2	−16.3	−0.9
208	−27.2	9.2	−22.3	9.6	18.3	21.7	−32.7	11.2	9.3	17.3
209	−6.0	16.2	2.8	22.1	20.4	24.6	−28.1	14.7	16.5	22.0
210	−10.5	14.8	1.4	20.1	22.3	25.9	−33.4	15.0	15.5	22.6
211	−4.9	16.0	3.5	20.0	21.9	25.5	−21.7	18.0	17.0	23.1
212	−20.0	−7.5	6.1	10.4	5.5	8.4	−78.4	−29.8	−19.5	−6.9
213	−40.8	−11.6	−31.6	−4.0	9.6	12.6	−45.5	−8.3	−0.3	6.5
214	−13.8	5.7	−0.3	17.4	15.4	19.5	−34.2	4.2	10.7	16.0
215	−21.8	−3.7	−5.8	9.2	13.8	16.8	−40.7	−3.2	6.6	12.1
216	−19.2	−0.7	−5.3	11.5	13.8	17.0	−34.7	−1.2	8.4	12.7
217	−19.9	−5.2	8.1	12.9	7.2	10.5	−83.4	−26.3	−18.4	−4.4
218	−42.4	−9.4	−33.1	−2.2	10.7	14.1	−48.1	−6.3	0.2	7.9
219	−11.8	10.0	1.0	20.8	17.9	22.4	−33.7	8.2	13.0	18.7
220	−18.1	4.1	−3.4	15.4	18.2	21.3	−37.3	3.0	10.4	16.6
221	−19.3	4.2	−4.2	15.7	18.6	22.4	−34.3	4.0	12.9	17.9
222	−14.0	7.3	12.9	18.5	14.2	18.0	−83.0	−3.6	−11.8	6.3
223	−40.9	−8.1	−32.1	−1.3	11.7	15.3	−47.2	−5.6	1.5	9.1
224	−5.0	20.1	2.8	23.9	23.7	28.3	−28.4	18.7	19.2	25.7
225	−18.0	1.6	−3.8	12.8	16.8	19.7	−35.7	0.2	8.9	14.7
226	−17.7	2.7	−3.8	14.1	17.6	21.4	−36.9	3.8	11.0	17.4
227	−21.2	−8.4	6.1	10.1	4.3	7.2	−83.2	−29.3	−20.4	−7.9
228	−39.4	−14.5	−30.8	−7.2	6.2	8.7	−42.4	−10.4	−2.4	3.2
229	−17.4	0.6	−5.9	10.7	10.2	13.3	−35.1	−1.5	5.0	9.9
230	−20.6	−3.8	−8.9	5.6	9.4	11.5	−32.5	−4.2	2.7	7.7
231	−20.8	−8.1	−5.2	5.7	8.3	11.2	−33.4	−4.6	3.5	7.7

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Table 5 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
232	−19.6	−6.3	7.6	11.7	6.3	9.2	−82.7	−26.9	−18.5	−5.7
233	−38.8	−7.3	−29.8	−0.7	12.0	15.3	−44.2	−4.2	2.6	9.6
234	−10.4	10.4	1.9	21.0	17.7	21.9	−32.5	8.9	13.2	18.7
235	−20.9	0.3	−7.2	11.1	16.0	18.7	−39.4	−0.1	8.6	14.4
236	−17.5	−0.6	−5.3	10.6	12.0	15.3	−31.6	−2.0	7.2	11.1
MAXD	−42.6	53.5	−33.1	55.5	54.1	63.6	−95.5	50.1	53.7	60.5
MD	−12.3	12.2	1.1	18.9	20.8	24.5	−32.2	9.0	12.4	19.6
MAD	16.0	15.5	10.5	19.4	20.8	24.5	33.8	17.5	17.9	20.4

Table 6: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the BP86-D3 functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−47.6	−2.9	−34.9	−2.9	−4.3	1.0	−43.4	−2.7	−7.0	−0.3
2	−55.3	−5.1	−40.5	−4.9	−6.5	−0.6	−49.6	−3.7	−9.4	−2.0
3	−49.2	−4.4	−36.4	−4.3	−4.7	0.7	−44.7	−3.7	−7.5	−0.7
4	−56.9	−5.0	−41.9	−4.9	−6.4	−0.4	−51.3	−3.6	−9.5	−1.8
5	−53.2	−4.6	−39.6	−4.7	−5.5	0.4	−48.6	−4.0	−8.6	−1.2
6	−57.5	−5.1	−42.6	−4.9	−6.5	−0.3	−52.2	−3.8	−9.6	−1.8
7	−53.0	−4.5	−39.5	−4.7	−5.2	0.4	−48.6	−4.0	−8.3	−1.1
8	−31.4	−11.6	−7.5	−1.8	−8.5	−4.2	−102.4	−31.1	−33.2	−15.1
9	−31.7	−10.5	−7.3	−1.2	−7.8	−3.4	−104.8	−28.2	−33.0	−13.9
10	−33.5	−19.2	−4.6	−0.1	−4.9	−1.6	−96.4	−36.5	−29.7	−15.3
11	−31.7	−16.7	−4.1	0.6	−3.8	−0.5	−96.3	−33.1	−28.7	−13.8
12	−31.0	−11.0	−7.3	−1.4	−7.9	−3.5	−102.6	−30.6	−32.6	−14.4
13	−30.2	−8.8	−5.9	0.4	−6.3	−1.8	−103.7	−26.8	−31.6	−12.2
14	−33.3	−18.9	−4.5	0.1	−4.9	−1.4	−96.5	−36.4	−29.6	−15.1
15	−31.9	−14.6	−4.1	1.0	−3.6	0.1	−99.0	−29.1	−28.9	−12.4
16	−30.4	−8.5	−6.6	−0.3	−6.7	−2.1	−103.8	−27.7	−32.1	−12.6
17	−30.0	−8.5	−5.7	0.8	−5.9	−1.4	−103.7	−26.6	−31.3	−11.8

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Table 6 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
18	−33.1	−18.1	−4.2	0.8	−4.4	−0.9	−96.6	−35.6	−29.4	−14.2
19	−32.2	−14.1	−4.4	1.0	−3.9	−0.1	−99.9	−28.3	−29.4	−12.1
20	−30.2	−8.2	−6.4	−0.1	−6.5	−1.9	−104.0	−27.5	−31.9	−12.3
21	−23.7	−4.4	−18.9	−4.3	−1.8	0.2	−27.0	−4.4	−4.8	−1.4
22	−28.2	−14.4	−20.3	−8.4	−2.9	−1.7	−28.0	−9.9	−5.6	−3.4
23	−24.8	−5.2	−20.1	−4.9	−2.0	0.0	−27.8	−5.5	−5.4	−1.9
24	−25.1	−5.4	−20.1	−4.9	−2.4	−0.7	−28.4	−5.5	−5.7	−2.4
25	−26.7	−6.0	−21.5	−5.7	−3.2	−1.2	−30.4	−6.2	−6.5	−2.9
26	−24.0	−5.0	−19.2	−4.7	−1.8	0.0	−27.2	−5.3	−5.0	−1.6
27	−23.8	−4.6	−19.2	−4.7	−1.8	0.2	−27.5	−5.0	−4.9	−1.5
28	−22.2	−2.9	−17.8	−3.1	−0.8	1.3	−25.5	−3.2	−3.7	−0.2
29	−25.0	−5.2	−20.3	−5.0	−2.0	0.0	−28.0	−5.5	−5.4	−1.9
30	−27.4	−5.6	−22.1	−5.8	−3.5	−1.4	−30.5	−6.1	−6.8	−3.0
31	−28.6	−11.2	−21.3	−7.3	−2.1	−0.7	−29.1	−7.6	−5.7	−2.7
32	−27.8	−5.2	−22.4	−5.3	−3.1	−1.0	−31.2	−5.4	−6.5	−2.5
33	−23.1	−3.8	−19.0	−4.2	−1.7	0.6	−26.7	−4.7	−4.7	−1.0
34	−21.6	−2.3	−17.3	−2.7	−0.3	1.8	−25.1	−2.9	−3.3	0.2
35	−24.2	−4.2	−19.5	−3.9	−1.0	1.0	−27.4	−4.6	−4.4	−0.8
36	−26.6	−3.5	−21.2	−3.7	−1.6	0.5	−30.1	−3.8	−5.1	−1.0
37	−21.8	−2.5	−17.7	−3.0	−0.4	1.9	−25.3	−3.5	−3.3	0.3
38	−35.8	−6.3	−28.4	−8.3	−7.6	−2.6	−60.9	−11.2	−13.9	−5.6
39	−39.6	−8.8	−29.8	−9.3	−10.2	−4.9	−67.7	−12.2	−16.9	−7.9
40	−36.3	−6.4	−28.6	−8.3	−7.3	−2.0	−62.0	−11.6	−13.6	−5.1
41	−41.4	−8.7	−31.3	−9.2	−10.2	−4.8	−70.5	−12.2	−17.3	−7.8
42	−35.9	−6.0	−28.4	−7.9	−6.9	−1.5	−62.2	−11.6	−13.2	−4.7
43	−41.8	−8.5	−31.7	−9.1	−10.3	−4.7	−71.3	−12.2	−17.4	−7.7
44	−36.1	−6.1	−28.7	−8.2	−7.0	−1.6	−62.5	−11.8	−13.3	−4.7
45	−43.7	−16.1	−37.4	−14.6	−14.4	−6.6	−60.3	−19.9	−15.3	−9.6
46	−40.9	−27.0	−35.2	−20.2	−12.4	−8.5	−53.3	−28.0	−14.7	−11.4
47	−32.4	−9.9	−25.6	−9.1	−7.6	−1.5	−44.7	−13.7	−8.5	−4.1
48	−50.7	−18.9	−43.2	−16.7	−17.6	−8.7	−67.7	−22.3	−18.1	−11.9
49	−49.2	−27.1	−40.8	−20.7	−14.6	−9.3	−60.7	−27.8	−16.8	−12.5

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Table 6 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
50	−37.1	−11.9	−28.5	−10.8	−9.2	−2.6	−50.5	−15.0	−10.0	−5.3
51	−42.8	−15.5	−35.7	−14.2	−13.0	−5.5	−58.4	−19.2	−13.9	−8.6
52	−53.3	−19.6	−45.3	−17.5	−18.9	−9.4	−70.1	−22.9	−19.4	−12.6
53	−51.7	−27.5	−42.8	−21.6	−15.5	−9.9	−63.8	−27.9	−17.9	−13.2
54	−39.0	−12.5	−29.7	−11.3	−9.7	−2.9	−52.4	−15.5	−10.7	−5.6
55	−41.4	−13.7	−34.4	−12.8	−12.4	−4.9	−56.2	−18.0	−13.1	−8.0
56	−42.5	−2.8	−26.6	−1.7	−7.1	−1.2	−50.1	−6.9	−9.8	−2.9
57	−50.9	−4.7	−32.7	−3.3	−9.8	−3.1	−58.1	−8.3	−12.4	−4.9
58	−42.7	−3.0	−27.0	−2.1	−7.3	−1.0	−50.4	−7.3	−9.8	−2.8
59	−46.8	−2.7	−31.1	−3.1	−9.7	−2.8	−56.8	−8.0	−12.3	−4.6
60	−42.7	−2.9	−27.2	−2.2	−7.1	−0.8	−50.6	−7.5	−9.7	−2.7
61	−53.9	−4.7	−35.1	−3.5	−10.3	−3.1	−61.7	−8.4	−13.2	−4.9
62	−42.6	−2.9	−27.1	−2.1	−7.1	−0.8	−50.6	−7.5	−9.6	−2.7
63	−32.7	−2.9	−24.8	−4.4	−7.5	−2.1	−59.1	−4.4	−11.9	−3.4
64	−68.5	−22.7	−50.2	−16.7	−10.8	−6.8	−58.6	−15.3	−14.7	−8.7
65	−64.9	−25.0	−47.9	−18.2	−11.4	−7.7	−54.5	−16.7	−15.0	−9.5
66	−68.3	−21.9	−50.6	−16.3	−10.5	−6.3	−59.1	−15.0	−14.4	−8.2
67	−62.8	−19.6	−46.8	−14.2	−9.6	−5.4	−54.2	−12.8	−13.1	−7.1
68	−64.8	−24.2	−47.9	−17.4	−10.9	−6.8	−54.8	−16.1	−14.4	−8.7
69	−69.0	−21.8	−51.7	−16.5	−11.0	−6.6	−60.4	−15.2	−15.1	−8.5
70	−64.0	−20.3	−47.8	−14.8	−10.1	−5.8	−55.5	−13.5	−13.5	−7.5
71	−65.0	−24.3	−48.5	−17.7	−11.2	−7.1	−55.6	−16.6	−14.7	−8.9
72	−68.5	−21.3	−51.3	−16.0	−10.5	−6.1	−60.0	−14.8	−14.5	−8.0
73	−63.6	−20.0	−47.6	−14.6	−9.9	−5.5	−55.5	−13.4	−13.2	−7.1
74	−65.1	−24.2	−48.7	−17.6	−11.2	−6.9	−55.8	−16.6	−14.7	−8.8
75	−35.1	−20.1	−6.0	−1.5	−5.5	−2.3	−103.3	−38.2	−30.7	−16.6
76	−34.1	−17.5	−6.0	−1.0	−5.2	−1.6	−102.7	−36.0	−30.5	−14.9
77	−34.2	−17.8	−7.5	−2.5	−6.5	−3.0	−100.8	−35.1	−31.2	−16.0
78	−34.1	−19.0	−5.6	−1.1	−4.9	−1.7	−102.3	−37.2	−29.9	−15.7
79	−34.0	−16.8	−6.2	−0.6	−5.1	−1.3	−103.0	−35.2	−30.6	−14.3
80	−33.1	−16.6	−6.5	−1.5	−5.5	−2.0	−99.6	−33.9	−30.0	−14.8
81	−34.2	−18.5	−5.9	−0.9	−5.1	−1.6	−102.5	−36.7	−30.2	−15.3

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Table 6 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
82	−33.2	−15.9	−5.5	0.1	−4.3	−0.5	−102.2	−34.4	−29.8	−13.4
83	−33.2	−16.6	−6.3	−1.0	−5.1	−1.6	−100.6	−34.5	−29.9	−14.3
84	−33.3	−17.6	−5.1	−0.1	−4.2	−0.7	−101.6	−35.9	−29.3	−14.3
85	−34.9	−16.9	−27.0	−13.7	−7.3	−6.7	−36.7	−14.1	−11.6	−8.9
86	−33.8	−16.5	−26.4	−13.4	−7.1	−6.5	−35.2	−13.6	−11.4	−8.8
87	−24.1	−10.9	−19.1	−8.7	0.1	0.8	−25.6	−9.7	−3.9	−1.5
88	−33.1	−16.7	−25.6	−13.5	−6.8	−6.2	−33.9	−13.9	−11.0	−8.6
89	−34.5	−16.4	−27.0	−13.5	−7.3	−6.6	−36.6	−14.0	−11.6	−8.8
90	−33.3	−15.3	−25.9	−12.7	−7.0	−6.3	−34.2	−12.7	−11.2	−8.5
91	−34.6	−16.4	−27.1	−13.5	−7.5	−6.6	−36.8	−14.0	−11.7	−8.8
92	−33.1	−15.1	−25.8	−12.5	−6.9	−6.1	−34.0	−12.5	−11.1	−8.3
93	−33.5	−16.1	−26.3	−13.2	−6.9	−6.2	−35.1	−13.5	−11.2	−8.5
94	−33.3	−16.0	−26.1	−13.2	−6.7	−6.2	−35.0	−13.5	−11.0	−8.4
95	−31.8	−13.0	−25.2	−10.8	−5.4	−4.7	−34.3	−11.0	−9.9	−6.9
96	−32.4	−14.3	−25.0	−11.6	−6.1	−5.3	−33.3	−11.7	−10.3	−7.4
97	−31.6	−12.5	−25.1	−10.4	−5.1	−4.4	−34.2	−10.5	−9.6	−6.5
98	−21.8	−8.3	−17.5	−7.0	1.2	2.1	−23.7	−7.5	−2.7	−0.2
99	−30.7	−13.5	−24.1	−11.1	−5.6	−4.7	−32.7	−11.6	−9.8	−6.9
100	−32.4	−14.8	−25.3	−12.0	−5.7	−5.0	−34.3	−12.4	−10.2	−7.3
101	−27.9	−12.9	−22.4	−10.5	−5.2	−4.5	−29.9	−11.6	−9.4	−6.6
102	−32.5	−14.5	−25.0	−11.7	−6.0	−5.2	−33.6	−12.0	−10.2	−7.4
103	−31.6	−12.0	−25.0	−10.1	−5.2	−4.3	−33.9	−10.0	−9.7	−6.4
104	−32.3	−14.4	−24.8	−11.7	−5.7	−5.2	−33.5	−12.0	−10.0	−7.3
105	−31.7	−15.3	−24.5	−12.2	−5.7	−5.0	−33.0	−13.0	−9.9	−7.3
106	−32.2	−14.8	−25.1	−12.1	−5.5	−5.0	−34.1	−12.5	−10.0	−7.3
107	−47.1	−22.3	−34.8	−16.1	−12.3	−8.7	−71.9	−22.5	−19.9	−12.6
108	−43.8	−24.7	−31.4	−15.7	−11.2	−8.3	−67.0	−24.5	−18.0	−12.2
109	−47.9	−21.5	−35.7	−15.6	−12.6	−8.5	−73.3	−22.3	−20.2	−12.4
110	−43.8	−18.5	−32.7	−13.7	−11.2	−7.4	−67.0	−19.1	−18.4	−11.0
111	−44.0	−23.3	−32.2	−15.1	−11.3	−7.9	−68.4	−23.7	−18.2	−11.8
112	−47.8	−20.5	−35.5	−14.9	−12.1	−8.2	−73.7	−21.7	−19.9	−11.9
113	−43.6	−18.4	−32.4	−13.6	−11.0	−7.2	−67.0	−19.1	−18.1	−10.8

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Table 6 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
114	−44.2	−22.5	−32.4	−14.7	−11.0	−7.4	−69.0	−23.1	−18.2	−11.3
115	−47.4	−20.2	−35.2	−14.6	−11.8	−7.8	−73.4	−21.4	−19.6	−11.6
116	−43.8	−18.6	−32.6	−13.7	−11.0	−7.3	−67.5	−19.6	−18.2	−10.8
117	−44.2	−22.4	−32.5	−14.6	−11.1	−7.4	−69.2	−23.1	−18.2	−11.2
118	−43.6	−25.0	−38.1	−20.8	−14.3	−10.0	−57.3	−26.2	−17.2	−13.3
119	−34.6	−16.1	−29.0	−14.5	−10.7	−5.8	−47.7	−19.5	−12.2	−8.8
120	−43.2	−26.5	−38.1	−21.3	−14.1	−9.8	−56.5	−27.3	−16.9	−13.1
121	−36.9	−17.3	−30.2	−15.4	−11.3	−6.6	−49.8	−19.7	−13.1	−9.5
122	−41.7	−22.2	−36.6	−18.6	−13.1	−8.1	−56.7	−23.5	−15.8	−11.5
123	−35.4	−15.1	−29.4	−13.2	−9.9	−4.8	−48.6	−18.8	−11.4	−7.8
124	−44.1	−25.1	−38.8	−21.3	−14.4	−9.9	−59.7	−26.0	−17.3	−13.2
125	−36.5	−14.8	−30.2	−13.7	−10.6	−5.7	−49.1	−17.8	−12.5	−8.7
126	−35.9	−15.5	−29.6	−14.2	−10.6	−5.6	−48.6	−18.5	−12.3	−8.6
127	−44.2	−23.1	−38.0	−19.5	−13.7	−8.7	−59.1	−24.3	−16.5	−12.2
128	−57.1	−18.8	−36.1	−12.6	−12.7	−8.2	−61.2	−18.2	−16.4	−10.4
129	−55.2	−20.2	−34.8	−13.4	−13.2	−9.0	−58.3	−19.0	−16.6	−11.1
130	−55.9	−17.6	−35.6	−11.7	−12.1	−7.1	−60.4	−17.3	−15.7	−9.4
131	−53.0	−16.1	−34.1	−10.6	−11.2	−6.5	−57.2	−15.6	−14.6	−8.5
132	−54.7	−19.4	−34.7	−12.8	−12.7	−8.2	−58.3	−18.5	−16.0	−10.3
133	−57.8	−18.0	−37.4	−12.4	−13.0	−7.7	−62.8	−17.9	−16.9	−10.1
134	−53.2	−16.4	−34.3	−10.8	−11.5	−6.7	−57.5	−15.8	−14.8	−8.7
135	−54.9	−19.3	−35.3	−12.9	−13.1	−8.2	−59.0	−18.6	−16.5	−10.4
136	−57.4	−17.6	−36.9	−12.0	−12.6	−7.4	−62.5	−17.6	−16.4	−9.7
137	−53.2	−16.3	−34.4	−10.8	−11.5	−6.6	−57.7	−16.0	−14.8	−8.6
138	−54.9	−18.9	−35.4	−12.7	−13.0	−7.9	−59.2	−18.4	−16.3	−10.1
139	−38.6	−16.9	−27.6	−11.8	−9.6	−6.2	−61.0	−15.6	−14.9	−8.4
140	−39.5	−15.4	−28.6	−10.7	−9.5	−5.6	−62.8	−14.9	−15.0	−7.8
141	−35.6	−13.5	−25.7	−9.6	−8.6	−5.2	−57.0	−12.9	−13.5	−7.2
142	−62.0	−32.7	−49.3	−23.5	−9.0	−7.3	−62.8	−28.7	−19.3	−12.9
143	−57.7	−31.1	−45.9	−21.8	−7.7	−5.8	−57.1	−25.8	−18.0	−11.8
144	−56.9	−31.6	−46.0	−22.2	−8.0	−6.1	−56.7	−26.2	−17.8	−11.8
145	−62.7	−34.9	−49.4	−25.1	−10.5	−8.8	−62.8	−30.5	−19.9	−13.9

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Table 6 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
146	−58.3	−33.2	−46.1	−23.5	−9.0	−7.4	−57.4	−27.6	−18.7	−13.0
147	−59.3	−34.4	−46.9	−24.1	−9.6	−7.8	−58.1	−28.3	−18.8	−13.1
148	−25.4	−16.5	0.2	3.5	−1.1	1.4	−78.6	−36.9	−23.9	−13.6
149	−38.6	−21.5	−13.5	−8.3	−14.9	−11.1	−109.6	−48.7	−40.0	−24.0
150	−50.2	−24.3	−39.9	−16.4	−2.9	−0.4	−53.2	−20.1	−11.7	−6.0
151	−40.5	−9.1	−40.0	−8.8	−4.7	0.2	−50.8	−10.9	−12.1	−3.7
152	−30.8	−15.5	−21.7	−7.5	−8.3	−5.0	−48.3	−17.3	−11.9	−7.6
153	−25.7	−5.5	−22.9	−6.1	−8.9	−4.3	−47.9	−14.6	−12.5	−6.9
154	−37.1	−21.4	−22.7	−9.5	−6.0	−3.3	−52.9	−20.5	−12.7	−7.6
155	−36.4	−16.1	−27.2	−10.1	−8.9	−5.1	−52.2	−17.6	−13.0	−8.2
156	−30.3	−9.1	−21.7	−6.1	−7.4	−3.4	−52.8	−12.7	−12.8	−6.2
157	−34.1	−11.9	−27.6	−9.9	−7.5	−3.2	−51.6	−16.0	−11.7	−6.6
158	−25.2	−16.3	0.2	3.5	−0.5	2.1	−78.5	−36.6	−23.4	−13.0
159	−25.5	−16.5	−0.1	3.2	−0.8	1.7	−79.0	−37.0	−23.8	−13.4
160	−49.7	−24.0	−39.7	−16.2	−2.2	0.2	−53.0	−20.0	−11.2	−5.5
161	−37.0	−5.0	−37.1	−5.2	−1.6	3.1	−45.5	−5.2	−9.2	−0.6
162	−31.4	−18.1	−21.2	−7.4	−6.7	−3.8	−45.1	−20.1	−10.9	−7.3
163	−28.8	−7.3	−24.0	−6.2	−8.7	−3.6	−51.3	−13.2	−12.0	−6.2
164	−37.5	−21.6	−24.2	−10.0	−5.7	−3.5	−50.1	−20.5	−12.3	−7.7
165	−34.7	−21.0	−23.6	−10.1	−8.2	−5.4	−48.1	−21.3	−13.0	−9.4
166	−37.2	−12.2	−26.0	−8.9	−7.5	−3.2	−60.9	−15.3	−14.1	−6.5
167	−41.3	−19.6	−30.4	−12.5	−10.0	−6.1	−57.8	−22.6	−14.5	−9.7
168	−25.1	−16.2	0.4	3.7	−0.1	2.5	−78.5	−36.4	−23.0	−12.6
169	−25.4	−16.3	0.1	3.5	−0.4	2.3	−79.4	−36.7	−23.4	−12.9
170	−50.5	−25.0	−40.2	−17.1	−3.9	−1.3	−53.0	−20.7	−12.7	−7.0
171	−56.1	−23.8	−48.9	−18.4	−7.5	−3.9	−63.5	−22.5	−17.1	−9.1
172	−33.3	−18.0	−21.6	−6.8	−9.0	−5.2	−52.2	−20.1	−13.0	−8.5
173	−36.1	−12.2	−28.7	−8.6	−10.7	−5.9	−59.3	−15.7	−14.8	−8.3
174	−34.9	−21.5	−23.8	−10.2	−7.8	−5.1	−47.9	−21.4	−12.4	−8.9
175	−44.2	−17.1	−30.4	−11.1	−9.0	−4.6	−67.8	−18.6	−16.1	−8.2
176	−43.6	−19.6	−31.8	−13.8	−11.8	−6.9	−63.4	−19.0	−16.6	−9.7
177	−24.6	−15.7	0.8	4.1	0.4	3.0	−77.7	−35.9	−22.5	−12.1

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Table 6 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
178	−36.6	−15.0	−11.8	−5.5	−11.8	−7.4	−111.1	−36.5	−37.2	−18.2
179	−50.2	−24.8	−39.9	−16.8	−3.6	−1.0	−52.8	−20.4	−12.4	−6.7
180	−50.5	−24.8	−40.6	−17.0	−2.9	−0.4	−54.0	−20.9	−11.9	−6.2
181	−38.4	−17.7	−27.7	−9.0	−11.3	−6.6	−60.3	−20.4	−15.2	−9.4
182	−38.5	−16.9	−28.2	−8.9	−11.5	−6.5	−60.9	−19.7	−15.2	−9.2
183	−36.2	−20.3	−22.9	−8.9	−4.5	−2.3	−48.8	−19.6	−11.1	−6.5
184	−34.3	−21.0	−23.1	−9.7	−7.3	−4.5	−47.2	−20.9	−11.9	−8.4
185	−42.3	−18.3	−28.6	−10.2	−8.1	−4.1	−65.1	−19.1	−15.1	−7.8
186	−42.0	−22.0	−29.5	−12.7	−10.4	−6.3	−59.7	−20.3	−15.4	−9.2
187	−34.1	−17.5	−5.6	−0.5	−5.9	−2.2	−100.8	−39.1	−31.8	−16.2
188	−59.4	−24.2	−51.2	−19.3	−7.7	−4.1	−67.4	−24.4	−17.8	−9.9
189	−45.0	−22.1	−33.5	−12.7	−15.5	−10.8	−68.4	−25.9	−20.4	−14.4
190	−51.7	−26.1	−37.1	−17.1	−14.1	−10.4	−75.9	−27.9	−22.3	−14.8
191	−50.1	−28.7	−37.0	−18.6	−15.7	−11.9	−69.6	−28.8	−22.1	−15.7
192	−35.0	−15.9	−5.9	−0.1	−5.7	−1.7	−104.7	−36.1	−32.2	−14.9
193	−60.9	−24.6	−53.0	−19.6	−8.2	−4.4	−69.6	−24.5	−18.5	−10.0
194	−47.3	−23.0	−35.5	−13.3	−16.9	−11.6	−71.8	−27.0	−21.5	−15.1
195	−54.4	−27.2	−38.2	−17.8	−15.3	−11.2	−79.7	−29.0	−23.5	−15.6
196	−53.5	−30.7	−39.1	−19.9	−17.5	−13.4	−74.1	−30.2	−23.7	−17.0
197	−33.5	−14.0	−5.6	0.1	−4.5	−0.6	−105.4	−29.4	−30.5	−12.9
198	−55.6	−14.8	−51.0	−14.9	−5.9	−2.0	−64.0	−14.5	−15.5	−6.5
199	−41.4	−14.5	−34.6	−11.2	−13.1	−7.8	−66.3	−17.7	−17.5	−10.6
200	−48.1	−16.7	−36.9	−14.1	−13.0	−8.5	−75.0	−18.1	−20.6	−11.9
201	−50.4	−19.2	−40.2	−15.6	−13.8	−8.9	−68.8	−20.6	−19.0	−12.4
202	−31.3	−16.8	−4.6	0.2	−5.1	−1.7	−90.7	−39.2	−30.5	−16.2
203	−61.4	−28.6	−52.1	−22.0	−9.0	−5.8	−66.7	−26.0	−19.4	−11.9
204	−41.6	−23.1	−30.2	−12.6	−13.1	−9.4	−59.5	−26.4	−18.4	−13.4
205	−47.7	−27.1	−32.6	−15.9	−12.3	−9.3	−67.4	−27.7	−20.3	−14.0
206	−47.9	−31.1	−33.8	−18.7	−14.7	−11.7	−64.1	−29.8	−20.8	−15.6
207	−34.5	−17.2	−6.7	−1.7	−6.8	−3.3	−101.4	−32.5	−31.6	−16.1
208	−51.8	−15.3	−46.8	−14.9	−6.2	−2.8	−57.3	−13.4	−15.3	−7.3
209	−40.5	−18.4	−31.7	−12.5	−14.1	−9.9	−62.6	−19.8	−18.0	−12.5

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Table 6 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
210	−45.4	−20.1	−33.6	−14.9	−12.6	−9.0	−68.4	−19.9	−19.5	−12.4
211	−39.0	−18.2	−30.6	−14.1	−12.2	−8.6	−55.9	−16.1	−17.1	−11.0
212	−30.3	−17.8	−4.2	0.1	−4.8	−1.9	−88.7	−40.0	−29.8	−17.2
213	−57.6	−28.4	−48.4	−20.8	−7.2	−4.2	−62.3	−25.1	−17.1	−10.4
214	−43.1	−23.7	−29.7	−12.0	−14.0	−9.8	−63.6	−25.2	−18.7	−13.4
215	−45.2	−27.1	−29.2	−14.2	−9.6	−6.6	−64.1	−26.6	−16.9	−11.3
216	−46.6	−28.2	−32.7	−15.9	−13.6	−10.4	−62.2	−28.7	−19.0	−14.8
217	−32.5	−17.8	−4.5	0.3	−5.4	−2.1	−96.0	−38.9	−31.0	−17.0
218	−62.1	−29.1	−52.8	−21.9	−9.1	−5.6	−67.8	−26.0	−19.5	−11.8
219	−45.5	−23.7	−32.7	−13.0	−15.9	−11.3	−67.4	−25.6	−20.7	−15.0
220	−49.0	−26.8	−34.3	−15.4	−12.7	−9.6	−68.2	−27.8	−20.5	−14.2
221	−51.4	−27.9	−36.3	−16.3	−13.5	−9.6	−66.4	−28.1	−19.2	−14.1
222	−33.4	−12.1	−6.5	−0.9	−5.2	−1.4	−102.4	−23.0	−31.2	−13.1
223	−60.7	−28.0	−51.9	−21.2	−8.1	−4.6	−67.0	−25.5	−18.4	−10.8
224	−42.9	−17.8	−35.1	−14.0	−14.2	−9.6	−66.4	−19.2	−18.7	−12.3
225	−43.8	−24.1	−29.6	−12.9	−9.0	−6.1	−61.5	−25.6	−16.9	−11.1
226	−50.6	−30.2	−36.7	−18.7	−15.3	−11.5	−69.8	−29.1	−21.8	−15.5
227	−31.6	−18.7	−4.3	−0.2	−6.0	−3.1	−93.6	−39.6	−30.8	−18.2
228	−52.3	−27.4	−43.7	−20.1	−6.7	−4.2	−55.3	−23.2	−15.3	−9.7
229	−40.4	−22.4	−28.9	−12.3	−12.8	−9.7	−58.1	−24.4	−17.9	−13.1
230	−37.1	−20.3	−25.4	−10.8	−7.0	−4.9	−48.9	−20.6	−13.7	−8.8
231	−40.5	−27.8	−24.9	−14.0	−11.4	−8.5	−53.1	−24.4	−16.2	−12.0
232	−30.7	−17.4	−3.5	0.6	−4.8	−1.9	−93.8	−38.0	−29.6	−16.7
233	−57.9	−26.4	−48.9	−19.8	−7.1	−3.9	−63.3	−23.3	−16.6	−9.5
234	−42.2	−21.4	−29.8	−10.8	−14.1	−9.8	−64.3	−22.9	−18.6	−13.1
235	−46.6	−25.4	−32.9	−14.6	−9.7	−7.0	−65.1	−25.8	−17.2	−11.3
236	−41.7	−24.8	−29.5	−13.6	−12.2	−9.0	−55.8	−26.2	−17.0	−13.2
MAXD	−69.0	−34.9	−53.0	−25.1	−18.9	−13.4	−111.1	−48.7	−40.0	−24.0
MD	−41.4	−16.9	−28.0	−10.2	−8.3	−4.6	−61.3	−20.1	−16.7	−9.4
MAD	41.4	16.9	28.0	10.4	8.3	4.9	61.3	20.1	16.7	9.5

Table 7: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the OLYP functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	1.6	53.8	17.1	56.7	55.8	63.2	7.7	54.2	50.8	61.1
2	−1.8	56.9	16.1	60.2	58.6	66.9	6.1	58.4	53.4	64.9
3	−0.4	51.9	14.9	54.7	54.4	61.9	6.1	52.9	49.5	59.9
4	−1.9	58.7	16.2	62.0	60.2	68.7	6.0	60.2	54.9	66.9
5	−0.6	56.0	15.7	58.9	57.9	66.1	6.0	56.9	52.6	63.9
6	−1.6	59.6	16.4	62.9	60.9	69.6	5.9	61.0	55.6	67.8
7	−0.2	56.4	16.1	59.2	58.4	66.4	6.2	57.1	53.1	64.2
8	12.7	35.0	37.4	45.4	38.4	43.9	−60.9	14.6	9.0	31.5
9	15.6	39.5	40.8	49.3	42.3	48.0	−60.0	20.7	12.1	36.0
10	−1.9	13.9	24.9	31.1	26.9	31.4	−66.0	−3.9	−1.7	15.9
11	2.2	18.8	28.1	34.5	30.6	35.1	−64.0	1.8	1.9	20.2
12	14.0	36.5	38.4	46.6	39.8	45.5	−60.0	16.1	10.4	33.2
13	17.7	41.9	42.6	51.5	44.2	50.1	−58.2	22.8	14.1	38.3
14	−1.4	14.5	25.1	31.4	27.0	31.6	−65.8	−3.5	−1.3	16.4
15	6.8	26.1	33.3	40.5	35.9	40.9	−62.2	10.8	6.4	27.0
16	17.7	42.5	42.5	51.3	44.0	50.0	−58.6	22.3	13.9	38.3
17	18.4	42.8	43.4	52.5	45.1	51.0	−57.7	23.7	14.9	39.3
18	−0.7	15.9	26.0	32.9	28.1	32.7	−65.4	−2.0	−0.7	18.0
19	8.4	28.7	35.0	42.6	37.5	42.7	−61.3	13.7	7.9	29.4
20	18.4	43.3	43.2	52.1	44.7	50.8	−58.2	23.1	14.7	39.1
21	43.9	66.7	48.9	68.3	71.9	74.0	40.5	66.5	64.1	70.2
22	18.3	34.0	24.7	40.3	47.9	49.1	17.9	37.9	40.1	44.2
23	45.1	68.6	50.1	70.3	74.3	76.3	42.1	68.1	65.8	72.3
24	42.0	65.4	46.9	67.1	70.9	72.6	38.6	65.1	62.5	68.7
25	43.6	68.2	49.1	70.0	73.6	75.6	40.2	67.9	65.3	71.9
26	41.9	64.3	46.5	65.7	69.8	71.7	38.7	63.8	61.9	68.0
27	43.9	66.7	48.6	68.0	71.9	73.9	40.3	66.1	64.1	70.2
28	45.9	68.9	50.6	70.0	73.4	75.6	42.6	68.3	65.8	72.0
29	46.1	69.8	51.0	71.3	75.3	77.4	43.2	69.2	67.0	73.4

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Table 7 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
30	46.5	72.7	52.2	73.9	76.9	79.1	43.5	71.8	68.8	75.6
31	31.5	51.8	37.9	56.5	63.2	64.7	30.4	54.7	54.7	60.2
32	47.6	74.5	53.3	75.9	79.0	81.2	44.4	74.0	70.5	77.8
33	47.1	70.2	51.8	71.3	74.8	77.2	43.7	69.1	67.3	73.7
34	46.8	69.8	51.4	70.8	74.1	76.3	43.2	68.9	66.5	72.8
35	47.7	71.6	52.5	73.2	77.1	79.2	44.5	70.9	68.7	75.3
36	50.8	78.3	56.5	79.7	82.5	84.7	47.4	77.7	74.0	81.5
37	48.9	72.0	53.6	73.1	76.5	79.0	45.5	70.9	69.2	75.6
38	37.4	71.7	48.6	72.4	71.6	78.0	10.6	66.3	60.9	73.8
39	39.7	75.8	53.0	77.6	75.4	82.4	9.6	71.7	64.0	78.0
40	37.8	72.5	49.1	73.2	72.6	79.3	10.7	67.0	62.0	75.2
41	41.5	79.8	55.3	81.8	79.2	86.3	10.7	75.8	67.3	82.1
42	38.8	73.5	49.9	74.1	73.5	80.3	11.2	67.7	63.0	76.3
43	42.9	81.8	56.6	83.7	80.7	88.1	11.6	77.6	68.9	84.0
44	38.9	73.7	49.9	74.2	73.6	80.5	11.2	67.8	63.3	76.6
45	47.5	81.4	58.1	85.8	86.7	96.0	29.2	76.4	82.2	91.3
46	7.9	24.7	15.1	32.7	42.3	46.9	−5.0	23.3	36.4	41.9
47	33.0	60.2	42.5	63.5	66.3	73.6	19.8	56.2	61.8	69.2
48	50.6	89.7	62.9	95.3	94.5	105.4	31.8	85.2	90.8	100.9
49	14.2	40.7	24.8	48.8	56.2	62.5	1.6	39.1	50.6	57.6
50	33.8	64.1	45.0	67.6	70.2	78.2	19.3	60.4	65.6	73.7
51	47.4	80.9	58.5	85.2	86.6	95.7	30.6	76.3	82.2	90.8
52	53.3	94.6	66.2	100.1	98.6	110.2	34.8	90.2	95.0	105.8
53	18.1	47.3	29.4	55.0	61.9	68.8	4.8	45.8	56.0	63.8
54	34.8	66.7	46.7	70.1	72.5	80.8	20.3	63.0	67.8	76.3
55	48.9	82.9	59.7	86.5	87.1	96.3	32.9	77.7	83.1	91.5
56	11.2	57.3	30.4	60.9	55.7	63.5	2.4	52.4	49.6	60.6
57	9.4	62.9	31.4	67.3	60.8	69.7	1.1	58.9	54.6	66.8
58	11.2	57.3	30.0	60.6	55.4	63.6	2.6	52.5	49.6	60.8
59	11.1	62.6	30.6	65.2	58.2	67.2	0.4	57.1	52.6	64.9
60	11.4	57.5	29.9	60.7	55.5	63.8	2.6	52.5	49.8	61.0
61	10.4	67.3	32.9	71.7	64.4	74.1	1.5	63.1	58.1	71.5

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Table 7 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
62	11.6	57.6	30.1	60.8	55.6	63.9	2.6	52.5	50.1	61.2
63	52.9	88.4	64.3	88.8	84.4	91.2	23.8	85.5	75.8	89.4
64	−22.2	29.7	−3.4	37.5	43.6	49.5	−11.6	36.3	36.7	46.4
65	−23.3	21.6	−6.2	29.9	37.1	42.6	−12.1	29.2	31.0	39.6
66	−21.4	31.4	−3.3	38.7	44.4	50.6	−11.6	37.4	37.6	47.6
67	−22.5	26.9	−5.7	34.5	39.2	45.2	−13.2	33.2	33.2	42.7
68	−22.5	23.2	−5.7	31.4	38.2	44.1	−11.9	30.6	32.2	41.2
69	−21.7	32.0	−3.9	39.2	44.5	51.0	−12.4	37.8	37.6	48.1
70	−23.0	27.0	−6.1	34.4	39.0	45.4	−13.7	33.2	33.4	43.0
71	−22.4	23.5	−6.0	31.6	38.1	44.2	−12.4	30.5	32.1	41.3
72	−21.0	32.7	−3.3	39.9	45.1	51.7	−11.9	38.4	38.4	48.9
73	−22.6	27.3	−5.9	34.7	39.2	45.7	−13.6	33.3	33.6	43.4
74	−22.2	23.9	−5.8	32.1	38.4	44.6	−12.3	30.9	32.6	41.8
75	3.3	19.6	29.7	35.7	32.8	37.1	−66.2	0.8	3.8	21.2
76	6.6	25.1	32.4	39.5	35.7	40.5	−64.2	5.2	6.1	25.5
77	4.4	22.8	29.3	36.2	32.4	37.2	−64.1	4.3	3.8	22.7
78	4.5	21.1	30.4	36.6	33.6	38.0	−64.9	2.2	4.9	22.5
79	7.2	26.6	33.1	40.9	36.4	41.5	−63.9	6.9	6.6	27.0
80	6.0	24.5	30.5	37.5	33.6	38.3	−62.4	6.0	5.3	24.3
81	4.9	22.2	30.7	37.5	34.0	38.6	−64.7	3.3	5.1	23.5
82	8.2	27.6	34.0	41.8	37.3	42.4	−62.9	8.0	7.6	28.1
83	6.1	24.7	31.0	38.4	34.2	39.0	−63.0	5.8	5.7	25.0
84	5.9	23.2	31.7	38.5	34.9	39.6	−63.7	4.3	6.2	24.6
85	14.5	35.5	20.8	38.9	46.2	46.9	11.6	37.2	37.3	42.4
86	21.2	41.6	27.4	44.9	52.5	53.2	18.9	43.3	43.7	48.6
87	24.0	39.6	28.3	42.2	52.4	53.1	21.3	39.6	44.3	48.8
88	20.6	39.7	26.5	42.9	50.9	51.5	18.7	41.2	42.4	47.0
89	14.8	35.9	20.8	38.9	46.0	46.7	11.6	37.1	37.1	42.3
90	20.4	41.9	26.7	44.6	51.3	52.1	18.4	43.1	42.4	47.6
91	14.7	36.1	20.7	39.0	45.9	46.8	11.5	37.3	37.1	42.4
92	20.5	41.9	26.7	44.7	51.3	52.1	18.4	43.2	42.4	47.6
93	22.0	42.5	27.9	45.4	53.0	53.7	19.4	43.9	44.2	49.2

Continued on next page

Table 7 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
94	22.1	42.5	28.1	45.4	53.1	53.7	19.5	43.9	44.4	49.2
95	18.4	40.9	24.0	43.5	49.6	50.4	14.8	41.6	40.3	46.0
96	21.5	43.1	27.7	45.7	52.2	53.1	19.4	44.3	43.4	48.8
97	18.8	41.7	24.4	44.2	50.3	51.1	15.1	42.5	40.9	46.7
98	24.8	40.8	28.6	42.7	51.9	52.9	21.9	40.6	44.4	48.9
99	21.7	42.1	27.2	44.8	51.3	52.2	18.7	42.8	42.6	47.8
100	23.1	43.8	28.9	46.7	54.2	55.0	20.2	45.1	45.3	50.5
101	23.2	41.1	27.6	43.5	50.1	50.9	20.2	41.4	41.8	46.8
102	21.3	42.8	27.5	45.5	52.2	53.1	19.1	43.9	43.4	48.7
103	20.3	43.8	26.0	46.0	51.6	52.6	16.8	44.4	42.3	48.4
104	21.5	42.8	27.7	45.5	52.4	53.1	19.2	43.9	43.6	48.7
105	22.7	41.9	28.4	44.8	52.5	53.2	20.4	43.1	44.2	49.0
106	23.4	44.0	29.3	46.8	54.4	55.0	20.5	45.2	45.7	50.6
107	16.3	44.6	30.4	52.0	55.3	60.1	−11.0	43.1	42.6	54.1
108	8.4	29.6	21.7	39.7	44.2	48.2	−16.5	29.3	32.8	42.0
109	17.6	47.8	31.6	54.8	57.2	62.6	−10.2	45.7	44.5	56.7
110	14.8	44.1	27.9	50.2	51.9	57.1	−10.9	42.0	40.1	51.7
111	10.9	34.1	23.8	43.5	47.0	51.6	−15.2	33.2	35.7	45.6
112	18.8	50.0	32.8	56.9	58.7	64.2	−9.6	47.5	46.0	58.5
113	15.3	44.6	28.4	50.5	52.2	57.3	−10.5	42.4	40.7	52.1
114	11.6	36.1	24.6	45.2	48.4	53.2	−14.9	34.9	36.8	47.5
115	19.2	50.3	33.2	57.2	59.0	64.4	−9.3	47.8	46.3	58.9
116	15.5	44.8	28.5	50.8	52.6	57.7	−10.5	42.4	41.0	52.5
117	11.9	36.6	24.8	45.6	48.6	53.6	−14.8	35.3	37.1	47.9
118	16.9	39.5	24.2	44.9	52.9	58.3	1.6	36.7	46.6	53.2
119	18.7	40.6	24.5	43.0	48.0	53.8	4.2	36.1	43.2	49.0
120	13.1	33.3	19.9	39.8	48.8	54.2	−1.5	31.3	42.8	49.1
121	19.0	42.3	26.3	45.1	50.3	56.0	4.8	38.7	45.0	51.2
122	20.9	44.6	27.6	49.5	56.2	62.3	3.9	41.6	50.1	57.4
123	17.5	41.7	23.7	44.5	49.1	55.4	2.9	36.9	44.6	50.8
124	17.2	40.4	24.4	45.6	53.4	59.1	−0.3	38.1	47.1	54.1
125	20.5	46.8	27.8	49.1	53.1	59.2	6.0	42.4	48.0	54.8

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Table 7 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
126	19.3	43.4	26.1	45.8	50.3	56.4	5.1	39.3	45.6	51.8
127	21.5	47.3	29.6	52.2	59.1	65.3	4.8	44.5	52.7	60.3
128	−10.6	32.9	11.7	40.7	40.8	47.0	−16.4	32.4	32.9	43.1
129	−12.8	26.6	8.4	34.9	35.2	41.0	−17.5	27.1	28.2	37.3
130	−9.8	33.7	11.6	41.1	40.7	47.4	−16.3	32.9	33.1	43.6
131	−11.8	30.4	8.7	37.9	37.4	43.7	−17.7	29.9	30.4	40.5
132	−11.7	28.0	9.0	36.0	36.1	42.4	−16.8	28.2	29.3	38.6
133	−9.7	35.7	12.2	43.0	42.2	49.4	−16.5	34.7	34.4	45.6
134	−12.0	30.1	8.4	37.5	36.7	43.3	−17.9	29.6	30.1	40.2
135	−11.5	28.7	8.9	36.6	36.2	43.0	−17.1	28.7	29.5	39.3
136	−9.1	36.2	12.7	43.5	42.6	49.8	−16.1	35.2	35.0	46.1
137	−11.5	30.7	8.7	38.1	37.1	44.0	−17.6	30.0	30.6	40.9
138	−10.9	29.6	9.4	37.4	36.9	43.8	−16.7	29.5	30.2	40.1
139	24.5	49.7	36.9	55.5	57.5	61.9	−1.0	49.3	47.6	58.2
140	26.9	54.8	39.3	60.4	60.9	66.0	0.6	53.7	50.9	62.6
141	23.3	49.2	34.8	53.9	54.4	58.9	−1.1	48.1	45.4	55.8
142	−23.9	9.3	−13.0	18.9	34.0	36.3	−26.4	12.1	18.5	28.2
143	−24.0	6.4	−13.8	15.9	31.3	33.6	−25.2	10.4	16.1	25.1
144	−22.9	5.9	−13.3	16.1	32.0	34.5	−24.0	10.5	16.8	25.8
145	−25.6	6.0	−14.6	15.6	31.5	33.7	−27.7	9.0	16.9	26.1
146	−25.8	3.1	−15.7	12.5	28.8	30.9	−26.9	7.0	14.3	22.7
147	−25.3	3.2	−14.7	13.7	30.5	32.7	−25.6	8.2	15.9	24.5
148	−5.3	4.7	18.1	22.3	19.4	22.8	−59.2	−16.1	−7.0	5.5
149	−3.1	16.4	22.5	29.6	23.1	28.1	−75.5	−11.0	−6.9	12.9
150	−20.1	7.7	−11.8	16.5	31.0	34.5	−23.2	12.4	16.0	25.2
151	11.8	48.3	12.2	50.2	54.6	61.1	1.2	46.4	41.6	54.7
152	6.4	23.9	15.3	32.6	32.5	36.9	−11.3	22.6	24.5	31.6
153	23.7	48.1	28.3	48.9	46.3	52.0	0.9	38.8	38.7	47.6
154	1.8	19.2	17.7	32.8	36.5	40.2	−14.6	20.6	24.9	32.9
155	11.9	35.7	22.6	43.2	45.4	49.9	−5.1	33.9	37.0	44.7
156	24.8	49.3	35.8	54.0	52.5	57.7	1.1	45.4	43.2	53.2
157	16.5	42.9	25.6	47.5	50.7	56.0	−1.3	39.3	42.0	50.5

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Table 7 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
158	−4.7	5.3	18.4	22.7	20.4	23.8	−58.7	−15.4	−6.0	6.5
159	−4.9	5.2	18.1	22.5	20.1	23.5	−59.2	−15.8	−6.4	6.2
160	−19.5	8.3	−11.4	16.8	31.7	35.2	−22.9	12.7	16.7	25.8
161	15.6	53.1	15.6	54.7	58.8	65.2	6.3	52.5	45.3	59.0
162	1.5	16.7	11.4	27.9	30.3	34.0	−12.0	15.4	20.7	26.9
163	26.4	52.0	32.5	54.4	51.9	58.4	3.4	46.0	44.1	53.7
164	−2.1	15.5	12.2	28.5	33.3	36.3	−15.0	17.1	21.5	28.9
165	0.5	16.4	12.5	28.6	32.0	35.5	−13.3	16.3	22.0	28.4
166	22.8	51.6	36.9	57.3	57.9	63.5	−2.1	48.4	46.6	58.3
167	8.4	34.0	20.7	42.6	46.3	51.1	−8.8	31.0	36.8	44.9
168	−4.3	5.8	18.8	23.2	20.9	24.5	−58.5	−14.9	−5.5	7.1
169	−4.3	6.1	19.0	23.5	21.1	24.6	−59.0	−14.7	−5.5	7.2
170	−21.5	6.1	−13.1	14.6	28.6	32.3	−24.2	10.7	13.9	23.0
171	−15.8	20.6	−10.3	27.1	38.0	43.0	−23.8	22.0	21.9	34.8
172	7.9	25.3	19.5	37.2	36.5	41.3	−11.1	23.9	26.8	34.4
173	21.5	49.7	29.8	54.5	52.6	58.9	−3.0	45.5	43.5	54.2
174	−0.5	15.0	11.4	27.4	31.2	34.7	−14.0	15.3	21.6	27.7
175	15.7	47.1	32.6	55.7	56.5	62.3	−9.3	45.6	44.1	56.7
176	16.7	44.9	30.7	52.1	53.8	60.0	−5.4	44.7	44.0	55.4
177	−3.8	6.2	19.2	23.5	21.3	24.8	−57.7	−14.5	−5.0	7.5
178	7.2	31.8	32.7	41.4	34.4	40.1	−69.7	9.6	3.9	27.6
179	−21.1	6.5	−12.7	15.0	29.0	32.7	−23.8	11.0	14.3	23.3
180	−20.0	7.9	−12.0	16.3	31.2	34.8	−23.5	12.1	16.2	25.4
181	13.6	37.8	24.6	47.4	45.7	51.8	−8.8	35.4	36.1	45.8
182	15.9	41.2	26.7	50.2	48.2	54.6	−7.0	38.7	38.8	48.9
183	−0.7	16.9	13.5	29.8	34.6	37.6	−13.5	18.2	22.9	30.2
184	0.1	15.4	11.8	27.7	31.5	35.0	−13.4	15.7	21.9	28.0
185	13.5	41.1	29.8	51.4	52.8	58.1	−10.4	40.4	40.4	52.1
186	9.1	32.3	22.8	42.5	45.2	50.5	−10.6	33.4	35.2	45.3
187	0.5	19.8	27.1	34.2	29.2	34.2	−69.5	−4.2	−1.1	18.2
188	−13.4	26.6	−7.3	31.5	43.1	48.3	−23.1	24.8	26.8	39.4
189	13.7	41.0	25.6	50.9	48.5	54.7	−11.4	36.1	37.9	47.9

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Table 7 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
190	11.3	41.1	28.4	51.5	53.7	58.7	−15.3	38.0	39.9	51.7
191	7.8	33.2	22.0	43.6	46.7	51.8	−14.6	31.2	35.2	45.4
192	3.9	26.3	31.4	39.6	33.9	39.4	−69.6	3.6	2.7	24.2
193	−13.7	27.7	−8.1	32.8	44.1	49.5	−24.0	26.4	27.4	40.8
194	15.0	44.2	27.1	54.1	50.8	57.7	−11.0	39.2	40.2	51.0
195	11.3	43.2	29.8	53.8	55.3	60.9	−16.3	40.1	41.5	54.0
196	7.1	34.1	22.6	45.2	47.7	53.2	−16.5	32.9	36.3	47.0
197	13.0	34.6	39.6	47.4	43.5	48.7	−61.0	18.2	12.8	34.8
198	−0.6	45.5	2.0	46.3	54.8	60.2	−10.6	44.5	39.3	53.8
199	26.7	58.4	34.1	62.8	60.9	67.7	0.2	54.2	51.0	62.6
200	28.2	64.4	42.4	68.9	69.5	75.4	−1.1	61.7	56.4	70.0
201	20.0	56.7	32.4	62.2	64.5	70.6	−0.2	54.0	54.2	65.0
202	−1.7	15.6	22.9	29.8	24.4	29.1	−64.4	−9.6	−4.3	13.1
203	−20.3	16.5	−13.6	22.7	36.0	40.6	−27.3	17.5	20.1	31.7
204	4.5	26.4	15.3	36.7	37.0	42.1	−14.7	22.2	27.1	35.3
205	4.0	27.8	20.4	39.8	43.1	47.4	−17.8	26.0	30.6	40.3
206	−0.6	19.0	13.5	31.0	35.8	39.9	−19.7	18.6	25.4	33.6
207	7.0	26.2	32.8	39.7	35.1	39.9	−62.0	9.7	6.5	25.7
208	−2.9	38.2	0.0	38.9	47.3	52.2	−10.1	38.7	33.3	45.8
209	19.3	45.2	27.9	51.4	50.1	55.7	−4.6	42.6	41.3	50.7
210	17.5	46.3	31.1	52.7	54.4	59.3	−8.0	45.2	43.1	54.1
211	18.4	42.9	28.0	47.4	49.6	54.5	−1.5	43.1	40.8	50.4
212	−4.5	10.3	19.3	25.3	21.2	25.2	−65.7	−14.3	−7.3	8.1
213	−23.0	9.5	−16.2	16.8	31.8	35.9	−29.1	11.6	16.0	26.4
214	7.8	30.6	21.1	42.5	41.9	47.3	−14.2	28.3	31.7	40.4
215	1.4	21.7	18.6	35.6	40.7	44.6	−19.4	21.5	28.6	37.1
216	−1.9	20.0	13.3	33.4	37.6	41.6	−19.2	18.3	27.1	34.2
217	−1.8	15.3	23.8	30.4	25.5	29.9	−67.9	−7.9	−3.9	13.2
218	−23.0	13.9	−16.3	20.9	34.6	39.4	−30.2	15.8	18.1	30.0
219	11.5	37.2	24.5	48.3	46.4	52.4	−11.9	34.6	36.0	45.5
220	5.4	31.1	21.2	43.2	46.2	50.3	−15.3	28.9	33.3	42.9
221	0.7	28.6	17.2	41.5	45.9	50.7	−16.0	27.4	35.0	43.4

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Table 7 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
222	15.4	39.1	41.5	49.4	45.1	50.2	−56.7	26.6	14.5	37.2
223	−21.4	15.3	−15.2	21.9	35.7	40.6	−29.2	16.5	19.4	31.3
224	22.2	51.6	30.5	56.5	56.3	62.3	−3.0	49.2	46.5	57.4
225	2.5	25.3	17.5	37.0	41.4	45.3	−16.5	23.2	29.2	38.0
226	5.5	29.3	20.2	41.1	45.1	50.0	−16.4	29.1	33.8	43.8
227	−4.9	9.8	19.9	25.4	21.0	24.8	−69.3	−13.1	−7.7	7.5
228	−24.2	3.1	−18.0	10.4	25.4	28.8	−28.7	6.4	11.1	19.8
229	−1.0	20.2	10.5	30.8	32.0	36.0	−20.0	17.6	21.2	29.2
230	−6.1	13.0	6.2	23.3	28.0	30.7	−18.8	12.3	17.0	24.4
231	−5.2	9.3	10.5	22.9	27.3	31.0	−20.3	11.3	17.9	24.5
232	−2.2	12.9	22.6	28.2	24.0	27.8	−67.6	−9.5	−4.7	11.0
233	−19.6	15.5	−12.6	22.5	36.2	40.7	−26.0	17.8	20.6	31.6
234	11.8	36.1	24.7	47.6	45.7	51.1	−11.6	34.1	35.2	44.3
235	2.6	26.8	17.7	38.9	44.3	47.8	−17.3	26.0	31.6	40.8
236	−2.8	17.2	10.5	29.5	33.0	37.0	−18.2	14.8	23.2	29.4
MAXD	53.3	94.6	66.2	100.1	98.6	110.2	−75.5	90.2	95.0	105.8
MD	9.9	38.2	23.6	45.6	48.0	52.8	−11.3	34.2	35.2	46.0
MAD	17.3	38.2	26.3	45.6	48.0	52.8	24.1	35.7	35.8	46.0

Table 8: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the PBE functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−30.8	17.7	−17.6	17.8	16.6	22.4	−26.3	17.6	13.0	20.9
2	−36.7	17.9	−21.2	18.1	16.7	23.1	−30.6	18.9	12.8	21.6
3	−32.7	15.9	−19.5	16.0	15.8	21.7	−28.0	16.3	12.2	20.1
4	−37.4	19.0	−21.8	19.1	17.6	24.3	−31.5	19.9	13.7	22.8
5	−34.8	17.9	−20.8	17.8	17.1	23.5	−30.0	18.1	13.1	21.8
6	−37.4	19.5	−21.9	19.6	18.1	24.8	−31.8	20.4	14.0	23.3
7	−34.4	18.2	−20.4	18.0	17.6	23.8	−29.8	18.3	13.7	22.1

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Table 8 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
8	−21.0	−0.2	2.4	8.8	2.0	6.5	−94.3	−20.9	−24.2	−4.6
9	−20.4	1.9	3.5	10.3	3.5	8.3	−95.9	−17.1	−23.2	−2.5
10	−28.2	−13.4	−0.4	4.5	−0.2	3.4	−93.2	−31.8	−26.4	−10.8
11	−25.8	−10.2	0.8	6.0	1.7	5.3	−92.6	−27.8	−24.6	−8.6
12	−20.1	0.9	3.1	9.6	2.9	7.6	−94.0	−20.0	−23.2	−3.5
13	−18.5	4.0	5.3	12.3	5.4	10.3	−94.4	−15.2	−21.4	−0.4
14	−27.7	−12.7	−0.1	5.0	0.1	3.8	−93.0	−31.4	−25.9	−10.3
15	−24.1	−6.0	2.8	8.5	3.9	7.9	−93.6	−21.8	−22.9	−5.0
16	−17.6	5.4	5.6	12.6	5.9	10.9	−93.5	−15.1	−20.9	0.2
17	−18.0	4.7	5.8	13.0	6.0	10.9	−94.1	−14.7	−20.8	0.3
18	−27.0	−11.5	0.6	6.1	0.9	4.7	−92.6	−30.1	−25.4	−9.0
19	−23.4	−4.4	3.5	9.5	4.5	8.7	−93.6	−19.9	−22.4	−3.7
20	−17.1	6.1	6.1	13.2	6.5	11.4	−93.4	−14.6	−20.3	0.8
21	0.4	21.4	5.0	21.3	24.2	26.2	−3.5	20.9	20.2	24.2
22	−16.0	−1.1	−8.6	4.6	10.8	12.0	−16.7	2.7	6.7	9.4
23	1.7	23.2	6.2	23.3	26.5	28.5	−1.8	22.4	22.1	26.3
24	−0.4	21.3	4.5	21.5	24.4	26.1	−4.2	20.6	20.0	24.0
25	−0.9	21.9	4.2	21.9	24.7	26.6	−5.0	21.0	20.4	24.7
26	0.0	20.8	4.6	20.8	24.0	25.8	−3.7	19.9	19.8	23.8
27	0.4	21.5	4.9	21.1	24.3	26.3	−3.7	20.5	20.3	24.3
28	2.8	23.9	7.1	23.4	26.0	28.1	−1.0	23.0	22.1	26.2
29	2.2	24.0	6.8	23.9	27.2	29.2	−1.3	23.1	22.8	27.0
30	1.3	25.4	6.6	24.8	27.4	29.5	−2.2	24.2	23.1	27.6
31	−9.2	9.7	−2.3	13.3	19.0	20.4	−10.5	12.6	14.3	17.8
32	0.5	25.3	5.8	24.8	27.3	29.4	−3.5	24.4	22.9	27.6
33	3.9	25.0	7.9	24.3	27.1	29.4	−0.1	23.6	23.3	27.5
34	3.8	24.9	7.9	24.2	26.9	28.9	−0.2	23.7	22.9	27.0
35	3.7	25.6	8.1	25.5	28.8	30.8	−0.1	24.6	24.3	28.6
36	2.9	28.2	8.1	27.6	30.0	32.1	−1.2	27.2	25.5	30.4
37	5.5	26.6	9.5	25.9	28.7	31.0	1.5	25.1	24.9	29.1
38	−5.4	26.5	3.0	24.6	25.1	30.5	−32.1	21.2	17.6	27.3
39	−6.7	26.8	4.1	26.4	25.2	31.0	−36.7	22.9	17.2	27.8

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Table 8 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
40	−5.2	27.0	3.3	25.3	26.0	31.6	−32.6	21.4	18.5	28.4
41	−6.7	28.8	4.4	28.4	27.0	32.9	−37.7	24.8	18.7	29.8
42	−4.4	27.9	3.9	26.0	26.8	32.5	−32.3	21.9	19.3	29.3
43	−6.0	30.2	5.0	29.5	28.0	34.1	−37.5	25.9	19.6	31.0
44	−4.5	28.0	3.8	26.0	26.8	32.6	−32.4	21.8	19.4	29.4
45	−1.1	29.7	6.3	31.3	32.5	40.6	−19.3	25.3	30.6	37.3
46	−20.3	−5.2	−14.7	1.7	10.4	14.4	−34.3	−6.7	6.8	10.8
47	−4.9	20.4	2.6	21.2	23.6	29.8	−18.5	16.0	21.6	26.8
48	−2.4	33.3	6.1	35.5	35.5	44.8	−21.1	29.3	34.0	41.4
49	−21.2	3.1	−12.6	9.4	16.6	22.0	−34.5	1.8	13.2	18.3
50	−7.2	21.0	2.1	22.2	24.5	31.4	−22.2	17.2	22.5	28.2
51	−1.2	29.3	6.9	30.8	32.9	40.8	−18.2	25.1	31.1	37.3
52	−2.0	35.7	7.0	37.8	37.2	47.2	−20.5	31.8	35.9	43.8
53	−20.4	6.3	−11.2	12.1	19.1	24.9	−34.4	5.1	15.6	21.2
54	−7.4	22.3	2.6	23.4	25.7	32.8	−22.4	18.6	23.6	29.7
55	0.3	31.3	8.4	32.4	33.6	41.5	−15.7	26.6	32.1	38.1
56	−21.4	21.9	−4.8	22.9	17.9	24.2	−30.3	17.0	13.9	22.1
57	−26.8	23.7	−7.8	25.0	18.9	26.0	−35.4	19.4	14.9	23.9
58	−21.4	21.9	−5.0	22.7	17.9	24.5	−30.3	17.0	14.1	22.4
59	−23.2	24.9	−6.7	24.6	18.2	25.5	−34.6	19.0	14.4	23.6
60	−21.2	22.1	−5.1	22.8	18.1	24.8	−30.3	16.9	14.3	22.7
61	−27.2	26.4	−7.8	27.5	20.8	28.6	−36.5	22.0	16.7	26.6
62	−21.0	22.2	−4.9	22.9	18.2	24.9	−30.3	17.0	14.5	22.8
63	5.1	37.7	13.9	36.0	32.7	38.4	−23.2	35.5	27.2	37.2
64	−54.0	−4.5	−35.7	1.4	7.6	12.1	−44.2	2.3	2.6	9.9
65	−52.8	−9.7	−35.9	−3.0	4.1	8.3	−42.5	−1.9	−0.5	6.1
66	−53.0	−2.8	−35.4	2.6	8.6	13.3	−44.0	3.5	3.6	11.1
67	−50.8	−4.2	−34.9	1.2	6.1	10.8	−42.5	2.1	1.6	8.7
68	−52.2	−8.3	−35.5	−1.7	5.1	9.6	−42.3	−0.8	0.5	7.4
69	−53.1	−2.1	−36.0	3.0	8.6	13.6	−44.8	3.8	3.5	11.3
70	−51.6	−4.3	−35.5	1.0	6.0	10.8	−43.4	1.9	1.6	8.9
71	−51.8	−7.8	−35.7	−1.5	5.1	9.8	−42.6	−0.7	0.6	7.6

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Table 8 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
72	−52.4	−1.4	−35.4	3.6	9.2	14.2	−44.3	4.4	4.2	12.0
73	−50.9	−3.8	−35.0	1.5	6.4	11.3	−43.0	2.2	2.1	9.4
74	−51.8	−7.5	−35.6	−1.2	5.3	10.1	−42.7	−0.5	0.9	7.9
75	−28.2	−12.7	−0.3	4.6	0.9	4.4	−99.0	−32.2	−25.7	−10.5
76	−25.0	−7.8	1.8	7.4	3.4	7.3	−96.3	−27.8	−23.4	−6.6
77	−26.3	−9.1	−0.7	4.9	1.0	4.9	−95.4	−27.9	−25.0	−8.6
78	−26.7	−10.9	0.7	5.7	2.1	5.6	−97.4	−30.6	−24.3	−8.9
79	−24.5	−6.5	2.1	8.3	3.9	8.0	−96.1	−26.5	−23.1	−5.4
80	−24.7	−7.4	0.7	6.3	2.3	6.2	−93.7	−26.3	−23.5	−7.0
81	−26.3	−10.0	0.8	6.3	2.3	6.0	−97.2	−29.7	−24.2	−8.1
82	−23.6	−5.5	2.9	9.1	4.7	8.9	−95.3	−25.5	−22.2	−4.4
83	−24.6	−7.3	1.1	7.0	2.8	6.7	−94.5	−26.7	−23.2	−6.4
84	−25.3	−9.0	1.7	7.2	3.2	7.0	−96.2	−28.7	−23.2	−7.1
85	−19.0	0.6	−11.8	3.4	10.2	10.9	−21.9	2.5	4.9	8.2
86	−15.2	3.9	−8.3	6.4	13.2	13.9	−17.4	5.8	7.9	11.1
87	−7.4	7.0	−2.8	8.8	18.3	18.9	−9.7	7.5	13.3	16.2
88	−14.7	3.2	−7.9	5.9	13.2	13.7	−16.4	5.1	7.9	10.9
89	−18.0	1.7	−11.2	4.0	10.7	11.4	−21.2	3.1	5.4	8.7
90	−14.5	5.2	−7.7	7.3	13.4	14.1	−16.4	6.9	8.0	11.5
91	−18.2	1.7	−11.3	4.0	10.5	11.4	−21.3	3.2	5.2	8.8
92	−14.3	5.4	−7.6	7.4	13.5	14.3	−16.2	7.1	8.1	11.6
93	−14.2	4.9	−7.6	7.1	14.0	14.7	−16.7	6.6	8.7	12.0
94	−14.0	5.0	−7.4	7.2	14.2	14.8	−16.6	6.6	8.9	12.0
95	−14.6	6.1	−8.6	7.7	13.4	14.2	−18.1	7.1	7.8	11.6
96	−13.4	6.5	−6.6	8.5	14.5	15.3	−15.3	8.1	9.2	12.7
97	−14.4	6.6	−8.5	8.1	13.8	14.5	−18.0	7.7	8.1	12.0
98	−5.0	9.8	−1.1	10.6	19.3	20.2	−7.7	9.8	14.5	17.5
99	−12.0	6.8	−6.1	8.6	14.5	15.4	−15.0	7.8	9.3	12.7
100	−12.8	6.5	−6.4	8.5	15.4	16.1	−15.7	7.9	9.9	13.3
101	−7.9	8.6	−3.1	10.3	15.9	16.6	−10.8	9.0	10.8	14.1
102	−13.3	6.4	−6.6	8.5	14.7	15.4	−15.5	7.9	9.4	12.8
103	−13.5	8.0	−7.5	9.2	14.5	15.5	−16.9	9.0	8.9	12.9

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Table 8 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
104	−13.2	6.5	−6.4	8.5	14.9	15.5	−15.3	7.9	9.5	12.9
105	−11.7	6.2	−5.2	8.6	15.6	16.3	−13.9	7.6	10.4	13.6
106	−12.5	6.6	−6.1	8.7	15.7	16.2	−15.4	8.0	10.2	13.5
107	−22.1	4.7	−9.4	10.8	14.7	18.6	−49.1	3.7	5.5	14.2
108	−25.4	−5.0	−12.8	4.1	8.7	11.9	−50.6	−5.5	0.4	7.4
109	−21.1	7.3	−8.5	13.0	16.1	20.5	−48.7	5.7	7.0	16.2
110	−20.6	6.7	−9.1	11.4	13.9	18.0	−45.9	5.2	5.2	14.0
111	−23.3	−1.1	−11.3	7.1	11.0	14.6	−49.7	−2.1	2.6	10.2
112	−19.8	9.5	−7.3	14.9	17.6	22.0	−48.0	7.5	8.4	17.8
113	−20.0	7.3	−8.5	11.9	14.4	18.5	−45.4	5.7	5.9	14.6
114	−22.6	0.6	−10.7	8.4	12.1	16.0	−49.4	−0.6	3.4	11.6
115	−19.3	10.0	−6.9	15.3	18.1	22.4	−47.6	7.9	8.8	18.2
116	−19.6	7.7	−8.2	12.3	14.9	18.9	−45.3	5.8	6.3	15.0
117	−22.4	1.1	−10.5	8.7	12.2	16.3	−49.3	−0.3	3.7	12.0
118	−15.2	5.4	−9.7	9.3	16.8	21.4	−30.7	3.4	12.8	17.6
119	−10.9	9.7	−5.6	10.8	15.4	20.4	−25.8	5.5	12.8	16.9
120	−17.7	0.7	−12.8	5.6	14.1	18.6	−32.9	−0.8	10.1	14.7
121	−12.8	9.1	−6.1	10.6	15.5	20.3	−27.6	5.8	12.5	16.9
122	−12.1	9.5	−7.2	12.7	19.1	24.4	−29.1	7.3	15.3	20.5
123	−11.4	11.3	−5.8	12.6	16.6	21.9	−26.5	6.7	14.1	18.5
124	−15.1	6.0	−9.9	9.5	17.3	22.1	−32.8	4.3	13.2	18.2
125	−11.1	13.4	−4.8	13.9	17.7	22.9	−25.5	9.4	14.7	19.5
126	−11.8	11.0	−5.7	11.9	16.1	21.3	−26.4	7.1	13.4	17.8
127	−13.1	10.4	−6.9	13.6	20.3	25.6	−29.9	8.3	16.4	21.7
128	−40.2	1.5	−18.8	7.6	7.9	12.8	−46.0	1.2	2.7	10.1
129	−40.6	−2.5	−20.0	4.2	4.7	9.2	−45.4	−2.2	−0.1	6.6
130	−38.8	2.8	−18.3	8.5	8.5	13.9	−45.1	2.2	3.4	11.1
131	−38.4	1.7	−19.2	7.1	7.0	12.0	−44.2	1.4	2.2	9.6
132	−39.4	−1.0	−19.3	5.3	5.8	10.6	−44.6	−1.0	1.1	8.0
133	−39.0	4.3	−18.4	9.6	9.3	15.0	−45.8	3.4	4.0	12.2
134	−38.3	1.8	−19.2	7.2	6.8	12.0	−44.2	1.4	2.2	9.6
135	−38.9	−0.2	−19.3	6.0	6.0	11.2	−44.7	−0.4	1.3	8.6

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Table 8 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
136	−38.4	4.9	−17.8	10.1	9.8	15.5	−45.3	3.9	4.6	12.8
137	−37.7	2.4	−18.8	7.7	7.3	12.6	−43.8	1.8	2.8	10.3
138	−38.5	0.6	−18.9	6.6	6.5	11.9	−44.5	0.2	1.8	9.3
139	−12.7	10.8	−1.3	15.8	18.1	21.8	−37.3	11.3	11.5	19.3
140	−10.5	15.4	0.6	19.9	21.0	25.3	−36.0	15.2	14.3	22.9
141	−10.8	13.1	−0.7	16.7	17.7	21.4	−34.4	12.9	11.6	19.2
142	−50.6	−19.2	−38.3	−10.0	5.3	7.2	−52.3	−15.8	−6.7	0.7
143	−47.9	−19.4	−36.5	−10.2	4.9	6.8	−48.2	−14.7	−7.1	0.0
144	−46.8	−19.7	−36.3	−10.1	5.1	7.1	−47.3	−14.6	−6.6	0.4
145	−51.7	−21.8	−39.0	−12.2	3.6	5.4	−52.9	−18.2	−7.6	−0.6
146	−49.1	−22.0	−37.4	−12.5	3.2	4.9	−49.1	−17.1	−8.1	−1.6
147	−49.6	−22.7	−37.5	−12.4	3.5	5.4	−49.1	−17.1	−7.6	−1.0
148	−24.3	−15.1	0.4	3.9	−0.4	2.3	−78.9	−36.3	−24.4	−13.4
149	−31.7	−13.7	−7.2	−1.4	−8.1	−4.0	−104.5	−41.9	−34.7	−17.4
150	−45.5	−18.1	−35.7	−9.9	4.5	7.2	−49.2	−13.9	−6.5	0.3
151	−22.1	11.8	−22.1	12.1	16.6	21.9	−33.3	9.7	7.5	17.4
152	−19.0	−2.5	−9.9	5.6	5.3	8.9	−37.7	−4.5	0.1	5.4
153	−5.5	16.7	−2.3	16.0	13.5	18.4	−28.8	7.3	8.7	15.3
154	−24.8	−8.0	−9.7	4.4	8.0	11.0	−41.7	−7.2	−0.3	5.8
155	−18.4	3.8	−8.8	9.9	11.8	15.7	−35.6	2.0	6.3	12.0
156	−8.5	14.4	0.7	17.4	16.1	20.4	−32.4	10.5	9.5	17.1
157	−14.5	9.9	−7.4	12.1	15.0	19.6	−33.5	5.3	9.5	15.6
158	−24.0	−14.7	0.4	4.0	0.3	3.1	−78.7	−35.9	−23.7	−12.7
159	−24.2	−14.9	0.2	3.8	0.0	2.8	−79.2	−36.3	−24.1	−13.0
160	−44.9	−17.6	−35.3	−9.6	5.2	7.9	−48.9	−13.7	−5.9	0.9
161	−18.7	15.9	−19.3	15.8	19.9	25.0	−28.2	15.4	10.5	20.7
162	−22.4	−8.0	−12.0	2.9	4.4	7.5	−36.9	−10.2	−1.6	2.9
163	−6.2	17.4	−1.2	18.3	16.1	21.6	−30.1	11.0	11.5	18.5
164	−27.4	−10.4	−13.5	1.7	6.1	8.6	−40.8	−9.4	−2.1	3.4
165	−23.0	−8.1	−11.7	3.1	5.5	8.5	−37.7	−8.9	−0.9	3.6
166	−13.6	13.4	−1.6	17.0	18.2	22.9	−38.8	9.9	10.2	19.1
167	−22.8	1.1	−11.5	8.4	11.5	15.5	−40.7	−2.4	5.3	11.2

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Table 8 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
168	−23.8	−14.5	0.7	4.3	0.8	3.6	−78.6	−35.6	−23.3	−12.2
169	−23.9	−14.4	0.6	4.3	0.7	3.5	−79.4	−35.7	−23.5	−12.3
170	−45.8	−18.7	−36.0	−10.6	3.3	6.1	−49.0	−14.5	−7.6	−0.8
171	−46.1	−11.4	−39.5	−5.9	5.5	9.4	−54.4	−10.4	−6.3	3.2
172	−18.7	−2.2	−7.0	9.2	7.6	11.6	−38.9	−4.5	1.7	7.2
173	−13.8	12.5	−6.2	15.9	14.2	19.4	−38.7	8.4	8.6	16.4
174	−23.8	−9.3	−12.4	2.4	5.3	8.2	−38.1	−9.6	−1.0	3.4
175	−21.7	7.8	−6.9	14.1	16.0	20.8	−46.8	5.9	7.2	16.6
176	−19.7	6.4	−7.4	12.2	14.8	19.9	−41.4	6.5	8.3	16.6
177	−23.2	−14.0	1.1	4.7	1.2	4.1	−77.8	−35.1	−22.8	−11.7
178	−26.1	−3.2	−1.8	5.2	−1.3	3.5	−102.8	−25.9	−28.3	−7.7
179	−45.5	−18.4	−35.7	−10.4	3.6	6.5	−48.7	−14.2	−7.2	−0.4
180	−45.6	−18.2	−36.0	−10.3	4.6	7.4	−49.6	−14.4	−6.5	0.4
181	−18.7	3.9	−7.9	12.6	10.7	15.8	−42.3	0.8	5.0	12.0
182	−17.7	6.0	−7.2	14.0	11.8	17.1	−41.7	2.9	6.3	13.6
183	−26.0	−9.1	−12.3	2.8	7.3	9.8	−39.5	−8.5	−0.8	4.6
184	−23.2	−8.8	−11.9	2.8	5.7	8.7	−37.4	−9.1	−0.5	3.9
185	−21.3	4.7	−6.8	13.0	14.9	19.3	−45.7	3.5	6.3	15.0
186	−22.5	−0.8	−9.7	8.5	11.3	15.8	−42.0	0.4	4.7	12.2
187	−26.4	−8.9	1.0	6.6	1.4	5.4	−95.7	−32.2	−25.9	−9.2
188	−45.7	−7.8	−38.2	−3.3	9.1	13.0	−55.0	−8.9	−3.2	6.2
189	−21.2	3.9	−9.7	13.1	11.0	16.0	−46.6	−0.8	4.2	11.5
190	−25.7	2.0	−10.3	11.1	14.1	18.2	−51.9	−0.5	4.2	13.1
191	−26.2	−2.9	−12.9	7.2	10.7	14.9	−47.7	−4.0	2.7	10.3
192	−25.3	−5.1	2.8	9.2	3.7	8.1	−97.7	−27.0	−24.3	−5.6
193	−47.0	−7.9	−39.9	−3.2	8.9	13.1	−57.0	−8.6	−3.6	6.4
194	−21.3	5.4	−9.4	14.8	11.9	17.5	−47.8	0.6	5.4	13.1
195	−26.9	2.6	−10.0	12.1	14.5	19.0	−54.3	0.0	4.6	14.0
196	−27.7	−2.9	−13.1	7.9	10.8	15.3	−50.5	−3.3	3.0	11.0
197	−22.1	−1.7	4.9	11.1	6.7	11.0	−96.8	−18.7	−20.9	−1.9
198	−38.6	5.3	−35.0	4.8	14.2	18.4	−48.5	4.8	2.6	13.4
199	−13.6	15.8	−7.0	18.7	17.3	23.0	−40.7	11.7	11.3	19.6

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Table 8 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
200	−16.0	18.0	−4.1	20.4	21.6	26.4	−45.1	15.7	12.4	22.6
201	−20.8	13.4	−10.3	16.8	19.2	24.4	−41.2	11.1	12.5	20.4
202	−25.5	−10.1	−0.1	5.4	0.1	3.9	−87.0	−34.1	−26.4	−11.2
203	−50.7	−15.5	−42.3	−9.3	4.5	8.0	−57.3	−13.8	−7.9	0.9
204	−24.6	−4.4	−13.4	5.8	6.0	10.1	−44.0	−8.5	−0.8	5.2
205	−27.9	−5.8	−12.4	5.5	9.2	12.6	−49.3	−7.0	−0.3	7.1
206	−29.8	−11.6	−15.8	0.7	5.4	8.7	−47.9	−11.2	−2.2	4.0
207	−26.0	−7.9	0.8	6.3	1.3	5.2	−95.5	−24.7	−24.9	−8.2
208	−37.7	1.6	−33.7	1.4	10.5	14.3	−44.5	2.7	−0.3	9.2
209	−17.4	6.9	−8.7	12.4	11.3	15.9	−41.4	4.7	5.9	12.6
210	−20.9	6.3	−8.7	11.4	13.7	17.7	−45.9	5.8	5.5	13.9
211	−15.5	7.2	−7.1	10.9	13.3	17.2	−34.4	8.4	7.1	14.3
212	−26.4	−13.1	−1.4	3.3	−1.4	1.8	−86.7	−36.9	−27.6	−14.1
213	−49.8	−18.5	−41.3	−11.2	3.6	6.8	−55.6	−15.8	−8.5	−0.6
214	−24.2	−2.9	−10.7	8.7	7.5	12.0	−46.5	−5.1	1.1	7.4
215	−30.1	−10.7	−13.5	2.6	7.4	10.7	−50.6	−10.7	−1.4	5.1
216	−30.1	−9.8	−15.7	2.7	5.9	9.3	−47.4	−11.1	−1.2	4.0
217	−26.6	−11.1	0.1	5.5	0.0	3.5	−92.3	−33.7	−26.9	−11.9
218	−52.0	−16.7	−43.6	−9.8	4.1	7.9	−59.0	−14.3	−8.5	0.5
219	−23.1	0.8	−10.2	11.4	9.2	14.1	−46.9	−1.8	2.6	9.5
220	−28.2	−4.1	−13.0	7.3	10.4	13.8	−49.0	−5.9	0.9	8.2
221	−32.1	−6.2	−16.5	5.5	9.3	13.4	−48.9	−7.2	1.9	8.0
222	−21.7	0.6	4.3	10.7	6.3	10.5	−93.6	−11.9	−21.3	−1.7
223	−50.4	−15.3	−42.5	−8.9	5.2	9.1	−57.9	−13.6	−7.2	1.8
224	−17.5	10.0	−9.7	13.5	13.8	18.8	−43.1	7.8	7.6	15.5
225	−26.6	−5.4	−12.1	5.8	10.0	13.2	−45.7	−7.4	0.7	7.5
226	−27.9	−5.7	−13.9	5.6	9.7	13.8	−49.1	−5.4	1.6	9.1
227	−27.8	−14.3	−1.6	2.9	−2.6	0.5	−91.9	−36.6	−28.7	−15.3
228	−47.4	−20.9	−39.4	−13.6	1.0	3.6	−51.3	−17.1	−9.7	−3.0
229	−26.7	−7.1	−15.1	3.1	3.5	6.9	−45.9	−9.6	−3.6	2.3
230	−27.6	−9.6	−15.7	0.0	4.1	6.3	−40.3	−10.3	−4.0	1.7
231	−28.9	−15.2	−13.1	−1.3	2.2	5.3	−43.1	−12.5	−4.1	0.9

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Table 8 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
232	−26.2	−12.2	−0.1	4.5	−0.7	2.5	−91.4	−34.2	−26.8	−13.0
233	−48.5	−14.7	−40.1	−8.2	5.5	9.0	−54.8	−12.1	−6.1	2.2
234	−21.4	1.4	−8.8	12.0	9.5	14.0	−45.2	−0.7	3.1	9.7
235	−30.1	−7.1	−15.6	4.0	9.3	12.2	−50.0	−7.9	0.1	7.1
236	−27.6	−9.1	−15.0	2.4	4.6	8.0	−43.0	−11.1	−1.8	2.8
MAXD	−54.0	37.7	−43.6	37.8	37.2	47.2	−104.5	−41.9	35.9	43.8
MD	−23.2	3.3	−10.0	9.7	12.0	15.9	−44.6	−0.6	2.2	10.5
MAD	23.5	11.3	12.1	11.4	12.1	15.9	44.6	13.4	12.0	13.3

Table 9: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the PBE-D3 functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−46.8	1.6	−33.7	1.7	0.6	6.4	−42.3	1.6	−3.0	4.9
2	−54.4	0.1	−39.0	0.4	−1.0	5.4	−48.4	1.1	−4.9	3.9
3	−48.6	0.0	−35.4	0.1	−0.2	5.8	−43.9	0.4	−3.7	4.2
4	−56.0	0.4	−40.3	0.6	−0.9	5.7	−50.1	1.4	−4.9	4.2
5	−52.2	0.4	−38.2	0.3	−0.4	6.0	−47.4	0.7	−4.4	4.3
6	−56.5	0.5	−41.0	0.6	−1.0	5.8	−50.9	1.3	−5.0	4.3
7	−52.0	0.6	−38.1	0.4	−0.1	6.1	−47.4	0.7	−4.0	4.5
8	−29.4	−8.6	−6.0	0.4	−6.4	−1.9	−102.7	−29.3	−32.6	−13.0
9	−29.6	−7.3	−5.7	1.1	−5.7	−0.9	−105.1	−26.3	−32.4	−11.7
10	−34.3	−19.5	−6.5	−1.6	−6.3	−2.7	−99.3	−37.9	−32.4	−16.9
11	−32.1	−16.5	−5.5	−0.3	−4.6	−1.0	−98.9	−34.1	−30.9	−14.9
12	−28.8	−7.8	−5.6	0.9	−5.7	−1.1	−102.7	−28.7	−31.9	−12.2
13	−28.1	−5.5	−4.3	2.8	−4.2	0.7	−103.9	−24.8	−30.9	−10.0
14	−34.0	−19.0	−6.4	−1.3	−6.2	−2.5	−99.3	−37.7	−32.2	−16.6
15	−31.5	−13.4	−4.7	1.0	−3.6	0.4	−101.0	−29.3	−30.4	−12.5
16	−27.4	−4.4	−4.2	2.8	−3.9	1.1	−103.3	−24.9	−30.7	−9.6
17	−27.8	−5.1	−4.1	3.2	−3.8	1.0	−103.9	−24.5	−30.7	−9.5

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Table 9 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
18	−33.8	−18.3	−6.2	−0.7	−5.9	−2.1	−99.4	−36.9	−32.2	−15.8
19	−31.4	−12.5	−4.6	1.4	−3.6	0.6	−101.6	−28.0	−30.5	−11.8
20	−27.1	−4.0	−3.9	3.2	−3.6	1.4	−103.4	−24.6	−30.3	−9.2
21	−18.0	3.0	−13.4	2.9	5.7	7.7	−21.9	2.5	1.8	5.8
22	−28.2	−13.3	−20.8	−7.5	−1.3	−0.1	−28.8	−9.4	−5.4	−2.7
23	−19.1	2.5	−14.5	2.5	5.8	7.7	−22.6	1.7	1.3	5.5
24	−19.8	1.9	−14.9	2.1	5.0	6.6	−23.6	1.2	0.6	4.6
25	−21.0	1.7	−16.0	1.7	4.5	6.5	−25.2	0.9	0.2	4.5
26	−18.7	2.0	−14.1	2.0	5.3	7.1	−22.4	1.2	1.1	5.1
27	−18.4	2.7	−13.9	2.3	5.6	7.6	−22.5	1.8	1.5	5.5
28	−16.2	4.9	−11.9	4.4	7.1	9.2	−19.9	4.1	3.2	7.3
29	−19.1	2.7	−14.5	2.6	5.9	7.9	−22.6	1.8	1.5	5.7
30	−20.8	3.3	−15.5	2.7	5.3	7.4	−24.3	2.1	1.0	5.5
31	−26.0	−7.1	−19.2	−3.6	2.1	3.6	−27.4	−4.3	−2.6	1.0
32	−21.4	3.3	−16.2	2.9	5.4	7.5	−25.4	2.4	1.0	5.7
33	−16.3	4.8	−12.2	4.2	7.0	9.3	−20.3	3.4	3.1	7.3
34	−15.4	5.7	−11.3	5.0	7.7	9.8	−19.4	4.5	3.8	7.9
35	−18.2	3.8	−13.7	3.7	6.9	8.9	−21.9	2.7	2.5	6.8
36	−20.0	5.3	−14.8	4.7	7.1	9.2	−24.1	4.3	2.6	7.5
37	−14.8	6.3	−10.8	5.6	8.4	10.7	−18.8	4.8	4.6	8.8
38	−27.0	4.9	−18.6	3.1	3.5	8.9	−53.7	−0.4	−4.0	5.7
39	−30.2	3.3	−19.5	2.8	1.6	7.4	−60.2	−0.6	−6.4	4.2
40	−27.3	5.0	−18.8	3.2	3.9	9.6	−54.6	−0.7	−3.6	6.3
41	−31.7	3.8	−20.6	3.4	2.0	7.9	−62.7	−0.2	−6.4	4.8
42	−26.9	5.5	−18.5	3.6	4.4	10.1	−54.7	−0.6	−3.1	6.9
43	−31.9	4.3	−20.9	3.7	2.1	8.2	−63.4	0.0	−6.3	5.1
44	−27.0	5.5	−18.7	3.5	4.3	10.1	−54.9	−0.7	−3.1	6.9
45	−34.8	−4.1	−27.5	−2.4	−1.2	6.9	−53.0	−8.4	−3.2	3.5
46	−39.5	−24.4	−33.9	−17.5	−8.8	−4.8	−53.5	−25.9	−12.4	−8.4
47	−30.2	−5.0	−22.7	−4.2	−1.8	4.4	−43.9	−9.4	−3.8	1.4
48	−41.2	−5.5	−32.7	−3.3	−3.3	6.0	−59.9	−9.5	−4.8	2.5
49	−46.7	−22.4	−38.2	−16.1	−9.0	−3.6	−60.0	−23.8	−12.4	−7.3

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Table 9 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
50	−34.6	−6.4	−25.3	−5.3	−2.9	3.9	−49.7	−10.2	−4.9	0.8
51	−34.5	−4.0	−26.5	−2.5	−0.4	7.4	−51.6	−8.2	−2.3	3.9
52	−43.0	−5.4	−34.1	−3.3	−3.8	6.1	−61.6	−9.3	−5.2	2.7
53	−48.6	−21.8	−39.4	−16.1	−9.1	−3.2	−62.6	−23.1	−12.6	−7.0
54	−36.3	−6.6	−26.2	−5.5	−3.1	3.9	−51.3	−10.3	−5.2	0.8
55	−33.3	−2.3	−25.2	−1.2	0.0	7.9	−49.3	−7.0	−1.5	4.5
56	−40.3	3.0	−23.6	4.1	−0.9	5.3	−49.1	−1.8	−4.9	3.3
57	−48.2	2.2	−29.2	3.5	−2.6	4.6	−56.9	−2.1	−6.6	2.5
58	−40.5	2.9	−24.1	3.7	−1.2	5.4	−49.3	−2.1	−4.9	3.4
59	−44.7	3.4	−28.2	3.1	−3.3	4.0	−56.1	−2.5	−7.1	2.1
60	−40.4	2.9	−24.3	3.6	−1.1	5.6	−49.5	−2.3	−4.8	3.5
61	−51.1	2.6	−31.6	3.6	−3.0	4.8	−60.4	−1.9	−7.2	2.7
62	−40.3	3.0	−24.2	3.6	−1.0	5.6	−49.5	−2.3	−4.7	3.6
63	−21.9	10.7	−13.2	8.9	5.6	11.4	−50.3	8.5	0.2	10.1
64	−69.0	−19.5	−50.7	−13.6	−7.4	−2.9	−59.2	−12.7	−12.4	−5.1
65	−65.9	−22.8	−48.9	−16.0	−9.0	−4.8	−55.5	−15.0	−13.5	−7.0
66	−68.8	−18.6	−51.2	−13.2	−7.2	−2.5	−59.8	−12.3	−12.2	−4.7
67	−65.1	−18.5	−49.2	−13.1	−8.1	−3.5	−56.7	−12.2	−12.7	−5.5
68	−65.9	−22.0	−49.2	−15.5	−8.6	−4.1	−56.1	−14.5	−13.2	−6.3
69	−69.5	−18.5	−52.4	−13.5	−7.9	−2.9	−61.2	−12.7	−13.0	−5.1
70	−66.2	−18.9	−50.1	−13.6	−8.6	−3.8	−57.9	−12.7	−13.0	−5.7
71	−66.1	−22.1	−49.9	−15.8	−9.1	−4.5	−56.9	−15.0	−13.6	−6.7
72	−69.0	−18.0	−52.1	−13.0	−7.4	−2.4	−60.9	−12.3	−12.5	−4.6
73	−65.8	−18.7	−49.9	−13.4	−8.5	−3.6	−57.9	−12.7	−12.8	−5.5
74	−66.2	−22.0	−50.0	−15.7	−9.1	−4.3	−57.1	−15.0	−13.5	−6.5
75	−34.9	−19.3	−6.9	−2.0	−5.8	−2.2	−105.6	−38.9	−32.4	−17.1
76	−33.1	−15.8	−6.3	−0.6	−4.7	−0.8	−104.4	−35.9	−31.5	−14.6
77	−33.9	−16.8	−8.3	−2.8	−6.7	−2.8	−103.1	−35.6	−32.7	−16.3
78	−33.8	−18.0	−6.4	−1.4	−5.1	−1.5	−104.5	−37.7	−31.4	−16.1
79	−33.1	−15.1	−6.5	−0.3	−4.7	−0.6	−104.7	−35.0	−31.7	−14.0
80	−32.6	−15.3	−7.2	−1.7	−5.6	−1.7	−101.7	−34.2	−31.4	−14.9
81	−33.8	−17.5	−6.7	−1.2	−5.2	−1.4	−104.6	−37.2	−31.7	−15.6

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Table 9 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
82	−32.2	−14.2	−5.7	0.5	−3.9	0.2	−103.9	−34.1	−30.8	−13.1
83	−32.8	−15.5	−7.1	−1.2	−5.4	−1.5	−102.7	−34.9	−31.4	−14.6
84	−32.9	−16.5	−5.9	−0.4	−4.4	−0.5	−103.7	−36.3	−30.7	−14.6
85	−33.8	−14.2	−26.6	−11.5	−4.6	−4.0	−36.7	−12.3	−10.0	−6.7
86	−31.1	−12.1	−24.3	−9.6	−2.7	−2.1	−33.4	−10.1	−8.1	−4.8
87	−21.5	−7.1	−16.9	−5.3	4.1	4.8	−23.9	−6.7	−0.8	2.0
88	−30.2	−12.3	−23.4	−9.7	−2.4	−1.8	−32.0	−10.4	−7.6	−4.6
89	−33.3	−13.7	−26.5	−11.3	−4.6	−4.0	−36.5	−12.2	−10.0	−6.6
90	−31.5	−11.7	−24.7	−9.7	−3.6	−2.8	−33.4	−10.0	−8.9	−5.5
91	−33.5	−13.6	−26.6	−11.3	−4.8	−3.9	−36.7	−12.1	−10.1	−6.6
92	−31.3	−11.6	−24.5	−9.6	−3.5	−2.7	−33.2	−9.9	−8.8	−5.4
93	−30.7	−11.6	−24.0	−9.3	−2.5	−1.8	−33.2	−9.9	−7.8	−4.5
94	−30.5	−11.5	−23.9	−9.3	−2.3	−1.7	−33.1	−9.9	−7.6	−4.4
95	−31.0	−10.4	−25.1	−8.8	−3.0	−2.3	−34.5	−9.4	−8.6	−4.9
96	−30.5	−10.7	−23.7	−8.7	−2.7	−1.9	−32.4	−9.0	−8.0	−4.5
97	−30.9	−9.9	−25.0	−8.4	−2.8	−2.0	−34.5	−8.8	−8.4	−4.6
98	−19.8	−5.1	−16.0	−4.3	4.5	5.3	−22.6	−5.0	−0.4	2.6
99	−28.8	−9.9	−22.9	−8.2	−2.2	−1.4	−31.7	−8.9	−7.5	−4.0
100	−29.6	−10.3	−23.2	−8.3	−1.5	−0.7	−32.5	−8.9	−6.9	−3.5
101	−25.2	−8.7	−20.4	−7.0	−1.4	−0.7	−28.0	−8.2	−6.5	−3.2
102	−30.6	−10.9	−23.9	−8.8	−2.6	−1.9	−32.8	−9.4	−7.9	−4.5
103	−30.6	−9.1	−24.6	−7.8	−2.5	−1.6	−33.9	−8.1	−8.1	−4.1
104	−30.5	−10.8	−23.7	−8.8	−2.4	−1.8	−32.6	−9.4	−7.8	−4.4
105	−28.6	−10.7	−22.2	−8.3	−1.4	−0.7	−30.9	−9.3	−6.6	−3.4
106	−29.4	−10.3	−23.0	−8.2	−1.2	−0.7	−32.3	−8.9	−6.7	−3.4
107	−41.4	−14.7	−28.7	−8.5	−4.7	−0.8	−68.5	−15.7	−13.8	−5.1
108	−40.9	−20.5	−28.3	−11.4	−6.8	−3.6	−66.1	−20.9	−15.1	−8.1
109	−41.9	−13.4	−29.3	−7.7	−4.6	−0.2	−69.4	−15.0	−13.8	−4.6
110	−39.7	−12.4	−28.2	−7.7	−5.2	−1.0	−65.0	−13.8	−13.9	−5.1
111	−40.5	−18.3	−28.5	−10.1	−6.2	−2.5	−66.8	−19.3	−14.6	−7.0
112	−41.7	−12.3	−29.1	−6.9	−4.2	0.2	−69.8	−14.3	−13.5	−4.1
113	−39.4	−12.2	−27.9	−7.5	−5.0	−0.9	−64.9	−13.8	−13.6	−4.9

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Table 9 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
114	−40.8	−17.5	−28.8	−9.7	−6.1	−2.2	−67.6	−18.8	−14.7	−6.5
115	−41.3	−12.0	−28.8	−6.6	−3.9	0.4	−69.6	−14.1	−13.2	−3.7
116	−39.6	−12.3	−28.2	−7.7	−5.1	−1.1	−65.3	−14.2	−13.7	−5.0
117	−40.8	−17.3	−28.9	−9.7	−6.2	−2.1	−67.7	−18.7	−14.7	−6.4
118	−40.5	−19.8	−35.0	−16.0	−8.4	−3.8	−56.0	−21.9	−12.4	−7.6
119	−33.1	−12.4	−27.7	−11.3	−6.8	−1.7	−47.9	−16.6	−9.4	−5.2
120	−41.5	−23.0	−36.5	−18.1	−9.6	−5.1	−56.6	−24.5	−13.6	−9.1
121	−35.0	−13.1	−28.3	−11.6	−6.7	−1.9	−49.8	−16.4	−9.7	−5.3
122	−38.8	−17.2	−33.9	−14.0	−7.6	−2.3	−55.8	−19.4	−11.3	−6.1
123	−35.4	−12.7	−29.8	−11.4	−7.4	−2.1	−50.5	−17.3	−9.9	−5.5
124	−41.4	−20.3	−36.2	−16.8	−9.0	−4.2	−59.1	−22.0	−13.1	−8.1
125	−35.8	−11.3	−29.5	−10.8	−7.0	−1.8	−50.2	−15.3	−10.0	−5.2
126	−34.9	−12.1	−28.7	−11.2	−6.9	−1.7	−49.4	−16.0	−9.7	−5.2
127	−41.3	−17.8	−35.1	−14.6	−7.9	−2.6	−58.1	−19.9	−11.8	−6.5
128	−57.0	−15.3	−35.7	−9.3	−8.9	−4.0	−62.8	−15.7	−14.2	−6.8
129	−55.5	−17.4	−34.9	−10.7	−10.2	−5.7	−60.3	−17.1	−15.0	−8.3
130	−56.1	−14.5	−35.6	−8.8	−8.8	−3.4	−62.4	−15.1	−13.9	−6.2
131	−54.6	−14.5	−35.4	−9.1	−9.2	−4.2	−60.4	−14.8	−14.0	−6.6
132	−55.1	−16.7	−35.0	−10.4	−9.9	−5.1	−60.3	−16.7	−14.6	−7.7
133	−57.8	−14.4	−37.1	−9.2	−9.5	−3.8	−64.6	−15.4	−14.8	−6.6
134	−54.8	−14.7	−35.7	−9.3	−9.7	−4.5	−60.7	−15.1	−14.2	−6.8
135	−55.3	−16.6	−35.7	−10.4	−10.4	−5.1	−61.1	−16.8	−15.1	−7.8
136	−57.4	−14.1	−36.7	−8.8	−9.1	−3.5	−64.3	−15.1	−14.3	−6.2
137	−54.8	−14.6	−35.8	−9.3	−9.7	−4.4	−60.9	−15.2	−14.2	−6.7
138	−55.2	−16.1	−35.6	−10.1	−10.2	−4.8	−61.2	−16.5	−14.9	−7.4
139	−32.7	−9.2	−21.4	−4.3	−2.0	1.7	−57.3	−8.7	−8.5	−0.8
140	−33.2	−7.2	−22.1	−2.8	−1.6	2.6	−58.7	−7.5	−8.3	0.2
141	−31.1	−7.2	−21.0	−3.6	−2.5	1.1	−54.6	−7.4	−8.7	−1.1
142	−61.8	−30.3	−49.4	−21.1	−5.8	−3.9	−63.5	−27.0	−17.8	−10.4
143	−58.0	−29.5	−46.6	−20.2	−5.1	−3.2	−58.2	−24.7	−17.1	−10.0
144	−57.1	−29.9	−46.5	−20.4	−5.1	−3.1	−57.6	−24.9	−16.8	−9.9
145	−62.8	−32.9	−50.0	−23.3	−7.5	−5.7	−64.0	−29.2	−18.6	−11.7

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Table 9 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
146	−59.1	−32.0	−47.4	−22.5	−6.8	−5.1	−59.1	−27.1	−18.1	−11.6
147	−59.8	−32.9	−47.7	−22.6	−6.7	−4.8	−59.3	−27.3	−17.7	−11.1
148	−27.8	−18.6	−3.2	0.4	−3.9	−1.2	−82.4	−39.8	−27.9	−16.9
149	−38.4	−20.3	−13.8	−8.0	−14.7	−10.6	−111.1	−48.5	−41.3	−24.0
150	−52.3	−24.9	−42.5	−16.7	−2.3	0.4	−56.0	−20.7	−13.3	−6.5
151	−37.4	−3.4	−37.4	−3.2	1.4	6.6	−48.6	−5.6	−7.7	2.1
152	−29.9	−13.4	−20.9	−5.3	−5.7	−2.1	−48.7	−15.4	−10.8	−5.5
153	−22.1	0.1	−19.0	−0.6	−3.1	1.8	−45.4	−9.4	−7.9	−1.4
154	−35.4	−18.6	−20.3	−6.2	−2.6	0.4	−52.3	−17.8	−10.9	−4.8
155	−34.0	−11.7	−24.4	−5.6	−3.7	0.2	−51.1	−13.6	−9.3	−3.5
156	−24.8	−1.9	−15.6	1.1	−0.2	4.1	−48.7	−5.8	−6.9	0.8
157	−32.1	−7.7	−25.1	−5.5	−2.6	2.0	−51.1	−12.3	−8.1	−2.0
158	−27.6	−18.3	−3.1	0.4	−3.3	−0.4	−82.3	−39.4	−27.3	−16.3
159	−27.8	−18.5	−3.4	0.2	−3.5	−0.8	−82.8	−39.9	−27.7	−16.6
160	−51.8	−24.4	−42.2	−16.5	−1.7	1.0	−55.7	−20.5	−12.8	−6.0
161	−34.4	0.2	−35.0	0.0	4.2	9.3	−43.9	−0.4	−5.2	5.0
162	−31.5	−17.1	−21.1	−6.2	−4.7	−1.6	−46.1	−19.3	−10.7	−6.2
163	−23.8	−0.2	−18.8	0.7	−1.5	4.0	−47.7	−6.7	−6.1	0.8
164	−36.7	−19.7	−22.8	−7.6	−3.2	−0.7	−50.2	−18.7	−11.4	−5.9
165	−34.3	−19.4	−22.9	−8.2	−5.7	−2.8	−49.0	−20.1	−12.2	−7.7
166	−31.9	−5.0	−19.9	−1.4	−0.2	4.5	−57.1	−8.5	−8.1	0.7
167	−39.4	−15.5	−28.1	−8.2	−5.1	−1.1	−57.3	−19.0	−11.3	−5.4
168	−27.4	−18.1	−2.9	0.6	−2.9	0.0	−82.2	−39.2	−26.9	−15.8
169	−27.7	−18.1	−3.1	0.6	−3.1	−0.2	−83.1	−39.5	−27.3	−16.1
170	−52.6	−25.5	−42.8	−17.5	−3.6	−0.7	−55.8	−21.3	−14.4	−7.6
171	−57.4	−22.8	−50.9	−17.3	−5.9	−1.9	−65.8	−21.7	−17.7	−8.2
172	−30.9	−14.4	−19.2	−3.1	−4.7	−0.7	−51.2	−16.7	−10.5	−5.0
173	−32.7	−6.4	−25.1	−3.1	−4.7	0.5	−57.6	−10.6	−10.4	−2.6
174	−34.6	−20.1	−23.2	−8.4	−5.5	−2.6	−48.9	−20.4	−11.8	−7.4
175	−40.4	−11.0	−25.6	−4.7	−2.7	2.0	−65.6	−12.9	−11.5	−2.2
176	−39.4	−13.3	−27.1	−7.4	−4.9	0.2	−61.1	−13.2	−11.4	−3.0
177	−26.9	−17.6	−2.5	1.1	−2.4	0.5	−81.4	−38.8	−26.4	−15.3

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Table 9 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
178	−35.0	−12.2	−10.7	−3.7	−10.2	−5.5	−111.7	−34.8	−37.2	−16.6
179	−52.3	−25.2	−42.5	−17.2	−3.2	−0.4	−55.5	−21.1	−14.1	−7.3
180	−52.6	−25.2	−43.0	−17.3	−2.4	0.4	−56.6	−21.4	−13.5	−6.6
181	−35.6	−13.0	−24.8	−4.3	−6.2	−1.1	−59.2	−16.1	−11.9	−4.9
182	−35.4	−11.7	−24.9	−3.7	−5.9	−0.6	−59.4	−14.8	−11.4	−4.1
183	−35.4	−18.5	−21.7	−6.5	−2.0	0.4	−48.9	−17.8	−10.2	−4.8
184	−34.0	−19.6	−22.6	−8.0	−5.0	−2.1	−48.2	−19.8	−11.3	−6.9
185	−39.0	−13.1	−24.6	−4.7	−2.8	1.6	−63.4	−14.2	−11.4	−2.7
186	−39.5	−17.9	−26.8	−8.6	−5.7	−1.3	−59.0	−16.7	−12.4	−4.9
187	−33.7	−16.2	−6.3	−0.7	−5.9	−1.9	−103.0	−39.5	−33.2	−16.5
188	−58.9	−21.0	−51.4	−16.4	−4.1	−0.2	−68.2	−22.1	−16.4	−7.0
189	−40.3	−15.2	−28.7	−5.9	−8.1	−3.0	−65.6	−19.8	−14.8	−7.5
190	−45.3	−17.5	−29.9	−8.5	−5.4	−1.4	−71.4	−20.1	−15.4	−6.5
191	−44.9	−21.6	−31.6	−11.6	−8.1	−3.9	−66.5	−22.7	−16.1	−8.5
192	−33.8	−13.6	−5.7	0.8	−4.8	−0.4	−106.2	−35.5	−32.8	−14.1
193	−60.6	−21.5	−53.6	−16.8	−4.7	−0.6	−70.6	−22.2	−17.2	−7.2
194	−41.8	−15.1	−30.0	−5.7	−8.7	−3.0	−68.3	−19.9	−15.1	−7.4
195	−47.5	−18.0	−30.7	−8.6	−6.1	−1.7	−74.9	−20.7	−16.1	−6.7
196	−47.9	−23.0	−33.2	−12.3	−9.3	−4.8	−70.6	−23.4	−17.2	−9.2
197	−31.3	−10.9	−4.3	2.0	−2.5	1.8	−105.9	−27.8	−30.0	−11.0
198	−54.1	−10.1	−50.5	−10.7	−1.3	3.0	−64.0	−10.7	−12.8	−2.1
199	−36.0	−6.5	−29.3	−3.6	−5.0	0.7	−63.1	−10.6	−11.0	−2.7
200	−39.8	−5.8	−27.9	−3.4	−2.2	2.6	−68.9	−8.1	−11.4	−1.2
201	−45.3	−11.1	−34.8	−7.6	−5.2	0.0	−65.7	−13.3	−11.9	−4.0
202	−31.9	−16.5	−6.4	−1.0	−6.3	−2.5	−93.4	−40.5	−32.8	−17.5
203	−61.7	−26.5	−53.3	−20.3	−6.5	−3.0	−68.3	−24.8	−18.9	−10.1
204	−39.3	−19.1	−28.1	−8.9	−8.6	−4.6	−58.7	−23.1	−15.5	−9.5
205	−43.5	−21.4	−28.1	−10.1	−6.4	−3.0	−64.9	−22.6	−15.9	−8.5
206	−44.9	−26.7	−30.8	−14.4	−9.6	−6.4	−63.0	−26.2	−17.3	−11.1
207	−33.6	−15.5	−6.9	−1.3	−6.3	−2.4	−103.1	−32.3	−32.5	−15.8
208	−50.5	−11.2	−46.5	−11.4	−2.2	1.5	−57.3	−10.1	−13.0	−3.6
209	−36.1	−11.8	−27.5	−6.3	−7.5	−2.9	−60.2	−14.0	−12.9	−6.2

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Table 9 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
210	−39.8	−12.6	−27.6	−7.5	−5.2	−1.2	−64.8	−13.1	−13.4	−5.0
211	−33.6	−10.9	−25.1	−7.2	−4.8	−0.8	−52.5	−9.6	−11.0	−3.7
212	−31.6	−18.3	−6.7	−1.9	−6.6	−3.4	−91.9	−42.1	−32.8	−19.3
213	−58.7	−27.4	−50.3	−20.1	−5.3	−2.1	−64.5	−24.8	−17.4	−9.5
214	−39.6	−18.3	−26.1	−6.8	−7.9	−3.4	−61.9	−20.6	−14.4	−8.0
215	−42.7	−23.3	−26.1	−10.0	−5.2	−2.0	−63.2	−23.4	−14.0	−7.5
216	−44.9	−24.6	−30.6	−12.2	−8.9	−5.5	−62.2	−26.0	−16.0	−10.8
217	−33.0	−17.5	−6.2	−0.9	−6.4	−2.8	−98.7	−40.1	−33.3	−18.3
218	−62.6	−27.3	−54.2	−20.4	−6.5	−2.8	−69.6	−24.9	−19.1	−10.1
219	−40.6	−16.8	−27.8	−6.2	−8.4	−3.5	−64.5	−19.3	−15.0	−8.1
220	−45.1	−21.1	−29.9	−9.6	−6.5	−3.2	−65.9	−22.9	−16.0	−8.7
221	−49.7	−23.9	−34.2	−12.1	−8.4	−4.3	−66.5	−24.9	−15.8	−9.6
222	−30.9	−8.6	−4.9	1.4	−2.9	1.2	−102.9	−21.1	−30.6	−11.0
223	−61.2	−26.0	−53.3	−19.6	−5.5	−1.7	−68.7	−24.3	−18.0	−9.0
224	−38.0	−10.5	−30.3	−7.0	−6.8	−1.8	−63.6	−12.7	−12.9	−5.0
225	−40.9	−19.7	−26.5	−8.6	−4.4	−1.2	−60.1	−21.8	−13.6	−6.9
226	−45.8	−23.7	−31.8	−12.4	−8.2	−4.1	−67.1	−23.4	−16.3	−8.8
227	−32.8	−19.3	−6.6	−2.1	−7.6	−4.5	−96.9	−41.6	−33.7	−20.3
228	−54.1	−27.5	−46.1	−20.3	−5.7	−3.0	−58.0	−23.8	−16.4	−9.7
229	−39.0	−19.4	−27.4	−9.2	−8.8	−5.4	−58.1	−21.9	−15.8	−9.9
230	−37.0	−19.0	−25.0	−9.4	−5.3	−3.0	−49.7	−19.6	−13.4	−7.6
231	−39.3	−25.7	−23.6	−11.8	−8.2	−5.1	−53.5	−22.9	−14.5	−9.6
232	−31.7	−17.7	−5.5	−1.0	−6.1	−3.0	−96.8	−39.7	−32.3	−18.5
233	−58.6	−24.8	−50.2	−18.3	−4.6	−1.1	−64.9	−22.2	−16.2	−7.9
234	−37.7	−15.0	−25.2	−4.4	−6.9	−2.4	−61.6	−17.1	−13.3	−6.6
235	−44.1	−21.1	−29.6	−10.0	−4.7	−1.8	−64.0	−22.0	−13.9	−6.9
236	−40.8	−22.3	−28.3	−10.9	−8.7	−5.2	−56.3	−24.4	−15.1	−10.5
MAXD	−69.5	−32.9	−54.2	−23.3	−14.7	11.4	−111.7	−48.5	−41.3	−24.0
MD	−39.1	−12.6	−25.9	−6.2	−3.9	0.0	−60.5	−16.5	−13.7	−5.4
MAD	39.1	13.6	25.9	7.4	5.1	3.3	60.5	17.0	14.0	7.3

Table 10: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the PW91 functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−34.5	15.3	−21.0	15.1	13.7	20.1	−30.0	15.1	10.4	18.6
2	−40.5	15.6	−24.8	15.5	13.7	20.8	−34.5	16.4	10.1	19.2
3	−36.3	13.6	−22.8	13.5	12.8	19.4	−31.7	13.8	9.6	17.8
4	−41.3	16.6	−25.4	16.4	14.5	21.8	−35.4	17.4	10.9	20.3
5	−38.5	15.5	−24.3	15.1	14.0	21.0	−33.8	15.6	10.4	19.4
6	−41.3	17.2	−25.6	16.9	14.9	22.4	−35.8	17.8	11.2	20.9
7	−38.2	15.9	−24.0	15.4	14.4	21.3	−33.6	15.8	11.0	19.7
8	−24.0	−2.6	−0.6	6.1	−1.3	3.8	−98.3	−23.8	−27.2	−7.2
9	−23.5	−0.6	0.4	7.6	0.1	5.5	−100.1	−19.9	−26.4	−5.1
10	−30.9	−15.7	−3.1	2.0	−3.2	0.9	−96.9	−34.4	−29.1	−13.2
11	−28.4	−12.4	−1.9	3.5	−1.3	2.8	−96.3	−30.3	−27.4	−11.0
12	−23.2	−1.6	0.0	6.8	−0.4	4.9	−98.1	−22.8	−26.3	−6.0
13	−21.6	1.6	2.1	9.5	1.9	7.5	−98.6	−18.0	−24.5	−3.0
14	−30.3	−15.0	−2.8	2.5	−2.9	1.3	−96.6	−33.9	−28.6	−12.6
15	−26.8	−8.3	0.0	5.9	0.8	5.3	−97.4	−24.3	−25.8	−7.5
16	−20.7	3.0	2.5	9.8	2.5	8.1	−97.7	−17.9	−24.0	−2.3
17	−21.1	2.3	2.5	10.2	2.5	8.0	−98.3	−17.4	−24.0	−2.3
18	−29.7	−13.9	−2.2	3.6	−2.2	2.1	−96.2	−32.6	−28.1	−11.3
19	−26.1	−6.7	0.6	6.9	1.3	6.1	−97.4	−22.4	−25.3	−6.1
20	−20.1	3.6	2.9	10.4	3.0	8.6	−97.6	−17.4	−23.4	−1.7
21	−3.3	18.7	1.5	18.4	21.3	23.6	−7.4	18.0	17.4	21.6
22	−19.0	−3.6	−11.6	2.1	8.3	9.7	−20.2	−0.2	4.2	7.0
23	−2.0	20.6	2.7	20.4	23.7	25.9	−5.8	19.4	19.3	23.7
24	−3.9	18.7	1.0	18.7	21.6	23.5	−8.1	17.7	17.3	21.5
25	−4.6	19.2	0.6	18.9	21.7	24.0	−9.1	18.0	17.4	22.0
26	−3.5	18.1	1.1	17.9	21.1	23.2	−7.6	16.9	17.1	21.3
27	−3.3	18.7	1.3	18.1	21.4	23.7	−7.7	17.5	17.4	21.7
28	−0.8	21.2	3.6	20.4	23.2	25.6	−4.9	20.1	19.3	23.7
29	−1.4	21.4	3.2	21.0	24.2	26.6	−5.3	20.1	19.9	24.4

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Table 10 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
30	−2.4	22.8	3.0	21.9	24.5	26.9	−6.2	21.3	20.3	25.1
31	−12.5	7.2	−5.6	10.5	16.2	17.8	−14.4	9.7	11.5	15.2
32	−3.3	22.5	2.0	21.8	24.3	26.7	−7.6	21.3	19.9	25.0
33	0.3	22.4	4.4	21.4	24.2	26.9	−4.0	20.7	20.5	25.0
34	0.1	22.2	4.4	21.3	24.0	26.4	−4.1	20.8	20.1	24.5
35	0.0	23.0	4.5	22.6	25.8	28.1	−4.1	21.6	21.4	26.0
36	−1.0	25.4	4.3	24.5	26.8	29.3	−5.4	24.1	22.5	27.7
37	1.9	24.0	6.0	23.0	25.7	28.5	−2.3	22.2	22.1	26.6
38	−9.4	23.6	−0.7	21.5	22.0	27.8	−36.7	18.2	14.5	24.5
39	−10.8	23.9	0.4	23.2	22.0	28.2	−41.5	19.9	14.0	25.0
40	−9.3	24.1	−0.3	22.1	22.9	28.9	−37.1	18.4	15.4	25.7
41	−11.0	25.8	0.5	25.1	23.7	30.0	−42.7	21.7	15.3	26.9
42	−8.5	24.9	0.3	22.9	23.6	29.8	−36.8	18.9	16.2	26.6
43	−10.4	27.1	1.0	26.2	24.5	31.2	−42.5	22.8	16.2	28.1
44	−8.6	25.0	0.1	22.8	23.6	29.8	−37.0	18.8	16.3	26.7
45	−6.1	26.1	1.7	27.5	28.7	37.5	−24.8	21.6	27.1	34.1
46	−23.5	−7.8	−17.9	−1.1	7.5	11.9	−38.3	−9.8	3.9	8.2
47	−9.5	16.9	−1.5	17.7	20.0	26.9	−23.5	12.4	18.5	23.9
48	−7.8	29.5	1.2	31.5	31.3	41.5	−27.0	25.4	30.3	38.1
49	−25.0	0.2	−16.4	6.3	13.3	19.2	−39.1	−1.5	10.0	15.5
50	−11.9	17.5	−2.2	18.5	20.7	28.3	−27.5	13.5	19.3	25.3
51	−6.1	25.8	2.4	27.0	29.1	37.7	−23.6	21.5	27.7	34.3
52	−7.5	31.9	2.0	33.7	32.9	43.7	−26.5	27.8	32.2	40.5
53	−24.5	3.3	−15.2	8.8	15.5	22.0	−39.2	1.7	12.3	18.3
54	−12.2	18.8	−1.8	19.6	21.8	29.6	−27.7	14.9	20.3	26.6
55	−4.6	27.7	3.9	28.6	29.7	38.4	−21.1	22.9	28.8	35.2
56	−25.3	19.3	−8.4	20.0	14.6	21.6	−34.7	14.1	11.3	19.8
57	−30.8	21.1	−11.6	22.0	15.4	23.4	−40.1	16.4	12.1	21.4
58	−25.3	19.4	−8.6	19.8	14.5	22.0	−34.7	14.1	11.5	20.1
59	−27.4	22.3	−10.6	21.6	14.7	22.9	−39.3	16.1	11.7	21.2
60	−25.1	19.5	−8.7	19.9	14.7	22.2	−34.7	14.1	11.7	20.3
61	−31.7	23.6	−12.0	24.2	16.9	25.7	−41.6	18.8	13.6	23.9

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Table 10 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
62	−24.9	19.6	−8.5	20.0	14.8	22.3	−34.6	14.1	11.9	20.5
63	0.7	34.5	9.8	32.5	29.1	35.3	−28.3	32.3	23.8	34.2
64	−57.0	−6.4	−38.7	−0.9	5.0	10.1	−47.6	0.0	0.2	7.7
65	−55.5	−11.5	−38.5	−5.0	1.7	6.4	−45.5	−4.1	−2.7	4.1
66	−56.2	−4.8	−38.4	0.3	5.9	11.2	−47.5	1.1	1.1	8.9
67	−54.0	−6.1	−37.9	−1.0	3.5	8.7	−45.9	−0.1	−0.8	6.6
68	−55.0	−10.2	−38.3	−3.9	2.6	7.6	−45.5	−3.1	−1.8	5.3
69	−56.3	−4.1	−39.1	0.6	5.8	11.4	−48.3	1.4	1.0	9.1
70	−54.7	−6.2	−38.4	−1.2	3.3	8.8	−46.7	−0.3	−0.7	6.8
71	−54.7	−9.8	−38.5	−3.7	2.5	7.7	−45.8	−3.0	−1.7	5.5
72	−55.7	−3.4	−38.6	1.3	6.4	12.0	−47.8	2.0	1.7	9.8
73	−54.0	−5.7	−38.0	−0.6	3.7	9.3	−46.4	0.0	−0.3	7.3
74	−54.7	−9.5	−38.5	−3.4	2.7	8.0	−45.9	−2.8	−1.5	5.8
75	−30.8	−14.8	−2.9	2.3	−2.0	2.0	−102.8	−34.7	−28.4	−12.7
76	−27.7	−9.9	−1.0	5.0	0.3	4.8	−100.2	−30.4	−26.2	−8.9
77	−28.8	−11.2	−3.3	2.6	−2.0	2.4	−99.2	−30.4	−27.8	−10.9
78	−29.2	−13.0	−2.0	3.3	−0.9	3.1	−101.2	−33.1	−27.0	−11.2
79	−27.2	−8.7	−0.7	5.8	0.8	5.5	−100.0	−29.0	−26.0	−7.8
80	−27.2	−9.5	−2.0	3.9	−0.6	3.7	−97.5	−28.8	−26.2	−9.3
81	−28.9	−12.1	−1.9	3.9	−0.8	3.6	−100.9	−32.1	−26.9	−10.4
82	−26.3	−7.7	0.1	6.7	1.6	6.3	−99.1	−28.0	−25.0	−6.7
83	−27.3	−9.4	−1.7	4.6	−0.2	4.2	−98.3	−29.1	−26.0	−8.7
84	−27.9	−11.1	−1.0	4.8	0.1	4.5	−99.9	−31.1	−25.9	−9.3
85	−22.0	−1.5	−14.8	0.9	8.0	8.7	−25.5	−0.1	2.4	6.0
86	−18.1	1.8	−11.2	4.0	11.0	11.8	−20.9	3.3	5.4	8.9
87	−10.2	4.9	−5.7	6.4	15.9	16.8	−13.0	4.9	10.9	13.9
88	−17.5	1.2	−10.7	3.6	11.0	11.6	−19.7	2.7	5.5	8.8
89	−21.0	−0.5	−14.2	1.6	8.3	9.2	−24.8	0.6	2.9	6.5
90	−17.5	3.2	−10.7	4.9	11.1	12.0	−19.9	4.5	5.6	9.3
91	−21.1	−0.4	−14.3	1.6	8.2	9.2	−24.9	0.6	2.7	6.5
92	−17.3	3.3	−10.5	5.0	11.2	12.1	−19.7	4.6	5.7	9.4
93	−17.1	2.8	−10.5	4.7	11.7	12.5	−20.2	4.1	6.2	9.8

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Table 10 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
94	−16.9	2.9	−10.3	4.8	11.9	12.6	−20.0	4.1	6.4	9.8
95	−17.7	3.9	−11.7	5.2	11.0	11.9	−21.7	4.5	5.3	9.3
96	−16.3	4.4	−9.5	6.1	12.1	13.1	−18.7	5.6	6.8	10.5
97	−17.5	4.4	−11.6	5.6	11.3	12.3	−21.6	5.1	5.5	9.7
98	−7.7	7.7	−3.9	8.2	17.0	18.0	−10.8	7.5	12.1	15.3
99	−15.0	4.7	−9.1	6.2	12.2	13.2	−18.4	5.3	6.8	10.5
100	−15.7	4.4	−9.4	6.1	13.0	13.9	−19.1	5.4	7.4	11.1
101	−10.7	6.5	−6.0	7.9	13.5	14.4	−14.0	6.6	8.4	11.9
102	−16.3	4.3	−9.5	6.1	12.3	13.2	−18.9	5.4	6.9	10.7
103	−16.6	5.8	−10.6	6.7	12.1	13.2	−20.5	6.4	6.4	10.7
104	−16.1	4.4	−9.3	6.2	12.5	13.3	−18.8	5.5	7.1	10.7
105	−14.5	4.2	−8.1	6.3	13.3	14.1	−17.2	5.2	8.0	11.4
106	−15.4	4.6	−9.1	6.3	13.3	14.0	−18.8	5.6	7.7	11.3
107	−25.6	2.1	−12.6	8.0	11.9	16.1	−53.5	0.8	2.7	11.7
108	−28.7	−7.7	−15.8	1.5	6.0	9.5	−54.7	−8.3	−2.4	4.9
109	−24.7	4.7	−11.9	10.2	13.2	18.0	−53.1	2.9	4.1	13.6
110	−24.0	4.3	−12.2	8.7	11.2	15.7	−50.0	2.6	2.4	11.5
111	−26.6	−3.8	−14.4	4.4	8.2	12.2	−53.8	−5.0	−0.2	7.7
112	−23.5	6.8	−10.7	12.0	14.7	19.4	−52.4	4.7	5.4	15.2
113	−23.3	4.9	−11.5	9.3	11.7	16.1	−49.5	3.1	3.1	12.2
114	−26.0	−2.0	−13.9	5.7	9.2	13.4	−53.6	−3.5	0.6	9.1
115	−22.9	7.3	−10.2	12.5	15.1	19.8	−52.0	5.1	5.9	15.7
116	−23.0	5.2	−11.3	9.6	12.1	16.5	−49.4	3.2	3.5	12.5
117	−25.8	−1.6	−13.7	6.0	9.3	13.7	−53.5	−3.1	0.8	9.5
118	−18.6	2.8	−13.1	6.4	14.0	19.0	−34.9	0.5	10.1	15.1
119	−14.5	6.9	−9.0	7.9	12.3	17.9	−30.0	2.4	10.0	14.4
120	−21.2	−2.0	−16.1	2.8	11.2	16.2	−37.1	−3.8	7.3	12.1
121	−16.4	6.5	−9.5	7.8	12.6	17.9	−31.7	2.9	9.8	14.5
122	−15.7	6.8	−10.8	9.7	16.1	21.8	−33.4	4.3	12.5	18.0
123	−15.5	8.1	−9.7	9.3	13.2	19.1	−31.2	3.2	11.0	15.7
124	−18.6	3.5	−13.2	6.6	14.4	19.6	−36.9	1.5	10.4	15.8
125	−15.0	10.5	−8.5	10.8	14.6	20.3	−30.0	6.3	11.9	16.9

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Table 10 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
126	−15.5	8.2	−9.2	8.9	13.1	18.8	−30.6	4.0	10.6	15.3
127	−16.8	7.7	−10.5	10.5	17.2	23.0	−34.4	5.2	13.5	19.1
128	−43.3	−0.5	−21.8	5.2	5.1	10.6	−49.8	−1.3	0.4	8.1
129	−43.4	−4.3	−22.7	2.0	2.1	7.2	−49.0	−4.5	−2.2	4.7
130	−42.0	0.8	−21.4	6.0	5.6	11.6	−49.0	−0.3	1.1	9.1
131	−41.5	−0.3	−22.2	4.8	4.1	9.8	−48.1	−1.1	−0.1	7.5
132	−42.3	−2.9	−22.1	3.1	3.0	8.5	−48.2	−3.4	−1.1	6.0
133	−42.3	2.2	−21.6	7.0	6.2	12.6	−49.8	0.8	1.6	10.1
134	−41.5	−0.2	−22.2	4.9	3.9	9.9	−48.1	−1.1	0.0	7.7
135	−41.9	−2.2	−22.1	3.7	3.1	9.1	−48.4	−2.8	−1.0	6.6
136	−41.8	2.7	−21.0	7.5	6.7	13.1	−49.4	1.3	2.2	10.6
137	−40.9	0.4	−21.8	5.4	4.3	10.4	−47.7	−0.6	0.5	8.3
138	−41.5	−1.4	−21.8	4.2	3.5	9.7	−48.1	−2.2	−0.5	7.3
139	−16.3	8.1	−4.7	12.8	15.1	19.1	−41.7	8.4	8.6	16.6
140	−14.3	12.6	−2.9	16.8	17.9	22.5	−40.5	12.2	11.3	20.2
141	−14.3	10.6	−3.9	13.9	14.8	18.8	−38.6	10.2	8.7	16.7
142	−53.5	−21.3	−41.0	−12.2	3.1	5.2	−55.9	−18.5	−9.2	−1.5
143	−50.9	−21.8	−39.4	−12.5	2.7	4.8	−51.8	−17.5	−9.6	−2.3
144	−50.0	−22.1	−39.2	−12.5	2.8	5.0	−51.1	−17.6	−9.1	−2.0
145	−54.3	−23.7	−41.5	−14.2	1.6	3.6	−56.2	−20.7	−9.9	−2.7
146	−51.8	−24.1	−40.0	−14.6	1.2	3.1	−52.6	−19.8	−10.4	−3.7
147	−52.5	−25.0	−40.2	−14.5	1.4	3.5	−52.7	−19.8	−10.0	−3.2
148	−26.7	−17.3	−2.0	1.7	−3.0	0.1	−82.1	−38.8	−26.6	−15.3
149	−34.9	−16.4	−10.3	−4.3	−11.4	−6.8	−108.3	−44.6	−37.7	−20.0
150	−48.4	−20.4	−38.2	−12.0	2.2	5.2	−52.7	−16.6	−8.9	−1.9
151	−25.5	9.5	−25.4	9.6	13.8	19.8	−37.2	7.0	5.1	15.3
152	−21.7	−4.6	−12.5	3.4	2.9	6.9	−41.1	−6.8	−2.2	3.3
153	−9.0	14.1	−5.6	13.3	10.8	16.1	−32.7	4.5	6.2	13.0
154	−28.0	−10.7	−12.4	2.0	5.5	8.7	−45.5	−10.1	−2.9	3.4
155	−21.6	1.4	−11.7	7.5	9.3	13.5	−39.3	−0.6	3.7	9.7
156	−11.9	11.8	−2.3	14.8	13.4	18.0	−36.2	7.8	6.7	14.7
157	−18.1	7.2	−10.6	9.4	12.2	17.2	−37.5	2.5	6.9	13.3

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Table 10 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
158	−26.4	−16.9	−1.9	1.8	−2.2	0.9	−81.9	−38.3	−26.0	−14.6
159	−26.7	−17.1	−2.2	1.6	−2.5	0.5	−82.4	−38.8	−26.4	−15.0
160	−47.7	−19.8	−37.9	−11.7	2.9	5.9	−52.4	−16.3	−8.3	−1.3
161	−22.0	13.6	−22.5	13.3	17.0	22.8	−32.1	12.8	8.1	18.6
162	−25.2	−10.3	−14.6	0.7	2.2	5.5	−40.4	−12.9	−3.8	0.8
163	−9.5	15.0	−4.3	15.7	13.5	19.4	−33.9	8.4	9.1	16.4
164	−30.6	−13.0	−16.3	−0.8	3.6	6.3	−44.7	−12.3	−4.7	1.0
165	−26.0	−10.6	−14.3	0.8	3.2	6.4	−41.4	−11.7	−3.3	1.4
166	−17.4	10.5	−4.9	14.1	15.3	20.3	−43.2	6.9	7.3	16.5
167	−26.4	−1.5	−14.7	5.7	8.6	13.1	−44.9	−5.3	2.6	8.7
168	−26.2	−16.7	−1.6	2.1	−1.8	1.4	−81.8	−38.1	−25.5	−14.1
169	−26.4	−16.6	−1.7	2.1	−1.9	1.2	−82.6	−38.2	−25.8	−14.3
170	−48.5	−20.9	−38.4	−12.7	1.0	4.1	−52.4	−17.1	−9.9	−2.9
171	−49.4	−13.8	−42.6	−8.3	2.7	7.1	−58.4	−13.2	−9.0	0.8
172	−21.6	−4.6	−9.7	6.8	5.2	9.5	−42.6	−7.2	−0.6	5.1
173	−17.3	10.0	−9.5	13.1	11.4	17.1	−42.9	5.7	5.9	14.0
174	−26.7	−11.7	−15.0	0.1	3.0	6.2	−41.7	−12.4	−3.4	1.2
175	−25.6	4.8	−10.3	11.1	13.0	18.1	−51.5	2.8	4.2	13.9
176	−23.1	4.0	−10.3	9.7	12.2	17.8	−45.4	3.9	5.7	14.4
177	−25.7	−16.2	−1.2	2.5	−1.4	1.8	−81.0	−37.6	−25.0	−13.6
178	−29.2	−5.8	−5.0	2.4	−4.8	0.6	−106.9	−28.6	−31.5	−10.3
179	−48.2	−20.6	−38.2	−12.5	1.3	4.5	−52.1	−16.9	−9.5	−2.6
180	−48.4	−20.4	−38.6	−12.4	2.3	5.4	−53.1	−17.1	−8.9	−1.8
181	−22.2	1.3	−11.1	9.9	7.8	13.4	−46.5	−2.1	2.4	9.7
182	−21.2	3.4	−10.5	11.2	8.9	14.7	−46.0	−0.1	3.7	11.2
183	−29.3	−11.8	−15.1	0.3	4.7	7.4	−43.3	−11.4	−3.5	2.2
184	−26.1	−11.2	−14.4	0.5	3.4	6.6	−41.0	−11.8	−2.9	1.7
185	−25.2	1.6	−10.2	10.1	11.8	16.6	−50.3	0.4	3.2	12.3
186	−25.6	−3.2	−12.5	6.1	8.8	13.6	−45.9	−2.3	2.1	9.9
187	−29.2	−11.2	−1.8	4.1	−1.5	3.0	−99.6	−35.1	−28.7	−11.4
188	−49.1	−10.2	−41.5	−5.8	6.3	10.6	−59.2	−11.9	−6.0	3.7
189	−24.8	1.3	−13.0	10.3	8.1	13.6	−51.0	−3.8	1.5	9.1

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Table 10 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
190	−29.6	−0.9	−13.8	8.0	11.0	15.4	−56.6	−3.8	1.1	10.3
191	−29.4	−5.3	−15.8	4.6	8.1	12.6	−51.9	−6.8	0.0	7.9
192	−28.2	−7.3	−0.1	6.7	0.6	5.6	−101.8	−29.8	−27.2	−8.0
193	−50.5	−10.3	−43.3	−5.8	6.0	10.7	−61.3	−11.6	−6.4	3.9
194	−25.0	2.8	−12.9	11.9	8.9	15.1	−52.3	−2.4	2.6	10.6
195	−30.8	−0.3	−13.5	9.0	11.4	16.3	−59.1	−3.2	1.4	11.2
196	−30.9	−5.2	−16.0	5.3	8.2	13.1	−54.6	−6.1	0.3	8.6
197	−25.0	−4.0	1.9	8.5	3.4	8.3	−101.0	−21.4	−23.9	−4.4
198	−42.0	3.1	−38.4	2.2	11.3	16.0	−52.7	2.1	−0.2	10.9
199	−17.3	13.3	−10.5	15.8	14.3	20.5	−45.2	8.9	8.6	17.2
200	−19.9	15.2	−7.8	17.3	18.4	23.7	−49.8	12.8	9.2	19.8
201	−24.7	10.8	−13.9	13.9	16.1	21.8	−45.8	8.2	9.6	17.9
202	−28.2	−12.4	−2.7	3.0	−2.7	1.5	−90.6	−36.9	−29.0	−13.3
203	−53.9	−17.9	−45.3	−11.7	1.9	5.8	−61.3	−16.7	−10.5	−1.5
204	−27.8	−6.9	−16.5	3.1	3.4	7.8	−48.1	−11.5	−3.4	2.8
205	−31.5	−8.6	−15.7	2.6	6.4	10.0	−53.7	−10.2	−3.2	4.4
206	−32.7	−14.0	−18.3	−1.7	3.1	6.7	−51.7	−14.0	−4.6	1.8
207	−28.8	−10.1	−2.1	3.7	−1.8	2.6	−99.5	−27.4	−27.8	−10.6
208	−40.9	−0.6	−36.8	−1.0	7.9	12.1	−48.2	0.2	−2.9	6.8
209	−20.7	4.5	−12.0	9.7	8.6	13.6	−45.5	2.1	3.3	10.3
210	−24.5	3.6	−11.9	8.6	10.9	15.1	−50.2	3.0	2.6	11.3
211	−18.4	5.1	−9.7	8.6	10.9	15.2	−37.9	6.1	4.7	12.2
212	−29.2	−15.5	−4.1	0.9	−4.2	−0.7	−90.5	−39.8	−30.2	−16.3
213	−52.8	−20.9	−44.2	−13.6	1.1	4.6	−59.5	−18.9	−11.0	−2.9
214	−27.5	−5.5	−13.8	6.0	4.9	9.8	−50.8	−8.2	−1.5	5.1
215	−33.6	−13.7	−16.6	−0.3	4.6	8.1	−55.1	−14.1	−4.3	2.4
216	−33.4	−12.4	−18.8	0.0	3.3	7.0	−51.7	−14.4	−3.8	1.6
217	−29.5	−13.6	−2.6	3.0	−3.0	1.0	−96.3	−36.6	−29.6	−14.2
218	−55.2	−19.1	−46.7	−12.2	1.5	5.6	−63.0	−17.3	−11.1	−1.8
219	−26.6	−1.8	−13.6	8.5	6.4	11.7	−51.4	−4.8	−0.1	7.1
220	−32.0	−7.1	−16.5	4.2	7.3	11.0	−53.6	−9.3	−2.2	5.4
221	−35.9	−9.0	−19.9	2.6	6.3	10.8	−53.5	−10.5	−0.9	5.5

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Table 10 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
222	−24.4	−1.6	1.4	8.1	3.1	7.9	−97.8	−14.6	−24.3	−4.2
223	−53.5	−17.6	−45.5	−11.3	2.6	6.8	−62.0	−16.5	−9.8	−0.6
224	−21.1	7.4	−13.3	10.5	10.7	16.3	−47.6	5.0	4.9	13.1
225	−30.1	−8.2	−15.4	2.9	7.1	10.6	−50.0	−10.6	−2.2	4.8
226	−31.1	−8.3	−16.8	2.9	7.0	11.4	−53.3	−8.4	−1.2	6.7
227	−30.8	−16.9	−4.4	0.3	−5.6	−2.2	−95.9	−39.6	−31.4	−17.6
228	−50.1	−23.0	−41.9	−15.6	−1.1	1.8	−54.8	−19.8	−11.8	−5.0
229	−29.9	−9.5	−18.0	0.7	1.1	4.7	−49.9	−12.5	−6.0	0.1
230	−30.9	−12.4	−18.6	−2.6	1.5	4.0	−44.2	−13.3	−6.6	−0.7
231	−31.4	−17.5	−15.3	−3.4	0.3	3.6	−46.6	−15.2	−6.2	−1.0
232	−29.1	−14.8	−2.9	1.9	−3.7	−0.2	−95.4	−37.2	−29.5	−15.4
233	−51.8	−17.2	−43.1	−10.6	2.9	6.8	−58.9	−15.0	−8.6	−0.1
234	−25.0	−1.4	−12.1	9.2	6.7	11.6	−49.7	−3.8	0.5	7.3
235	−33.9	−10.2	−18.9	1.1	6.4	9.6	−54.6	−11.3	−2.9	4.3
236	−30.9	−11.8	−17.9	−0.1	2.1	5.8	−47.1	−14.2	−4.3	0.5
MAXD	−57.0	34.5	−46.7	33.7	32.9	43.7	−108.3	−44.6	−37.7	40.5
MD	−26.5	0.8	−13.1	7.0	9.1	13.5	−48.6	−3.4	−0.5	8.1
MAD	26.5	10.9	13.8	9.3	9.7	13.6	48.6	13.3	11.3	12.0

Table 11: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the TPSS functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−20.5	23.9	−8.1	24.0	21.5	28.2	−15.9	24.1	20.4	27.4
2	−25.0	25.0	−10.5	25.2	22.3	29.8	−18.8	26.3	21.1	28.8
3	−22.2	22.3	−9.7	22.5	20.7	27.6	−17.4	22.9	19.8	26.7
4	−25.5	26.2	−10.7	26.4	23.4	31.1	−19.3	27.5	22.2	30.2
5	−23.6	24.7	−10.3	24.6	22.4	29.8	−18.5	25.2	21.1	28.8
6	−25.3	26.8	−10.7	27.0	23.9	31.8	−19.5	28.0	22.6	30.8
7	−23.1	25.1	−9.9	24.9	23.0	30.2	−18.3	25.5	21.7	29.2

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Table 11 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
8	−11.1	6.9	10.8	16.3	7.4	12.6	−78.6	−12.1	−12.8	3.6
9	−10.2	9.0	12.2	18.1	9.2	14.7	−79.7	−8.3	−11.4	5.9
10	−17.3	−4.5	8.8	13.0	6.2	10.3	−76.5	−21.0	−14.3	−1.3
11	−15.5	−2.1	9.5	13.9	7.5	11.6	−76.2	−17.6	−13.1	0.3
12	−10.5	7.7	11.3	16.9	8.2	13.6	−78.5	−11.4	−12.0	4.6
13	−8.5	11.0	13.9	20.0	10.9	16.6	−78.3	−6.6	−9.7	7.9
14	−16.8	−4.0	9.1	13.5	6.5	10.7	−76.3	−20.6	−13.8	−0.8
15	−13.7	1.9	11.6	16.5	9.7	14.3	−76.9	−11.9	−11.3	3.7
16	−7.9	12.0	13.9	19.8	11.2	16.9	−77.7	−6.6	−9.5	8.2
17	−7.9	11.7	14.5	20.7	11.6	17.2	−78.0	−6.0	−9.1	8.7
18	−16.2	−2.8	9.8	14.6	7.3	11.7	−75.8	−19.3	−13.2	0.5
19	−13.0	3.3	12.3	17.5	10.3	15.1	−76.8	−10.1	−10.7	5.0
20	−7.4	12.6	14.3	20.4	11.7	17.4	−77.6	−6.2	−9.0	8.8
21	10.8	29.3	15.2	29.8	31.6	34.0	8.2	29.6	29.3	32.8
22	−5.3	7.7	1.8	13.6	18.2	19.6	−5.0	11.9	15.5	17.9
23	12.5	31.6	16.9	32.2	34.4	36.8	10.1	31.5	31.6	35.3
24	10.0	29.1	14.7	29.9	31.7	33.8	7.4	29.2	29.0	32.6
25	10.0	30.1	14.8	30.6	32.4	34.8	7.2	30.0	29.7	33.5
26	10.0	28.3	14.5	28.9	31.0	33.2	7.4	28.2	28.6	32.0
27	10.7	29.2	15.0	29.5	31.7	34.1	7.8	29.0	29.3	32.8
28	12.7	31.4	17.0	31.5	33.3	35.7	10.2	31.3	31.0	34.6
29	13.0	32.3	17.3	32.8	35.0	37.4	10.6	32.1	32.3	36.0
30	12.1	33.5	17.1	33.5	35.1	37.6	9.8	33.1	32.7	36.6
31	2.1	18.6	8.7	22.6	26.9	28.6	2.0	22.2	23.7	26.8
32	11.9	33.7	16.9	34.0	35.5	38.0	9.2	33.7	32.9	37.0
33	13.6	32.3	17.7	32.4	34.1	36.9	10.8	31.8	32.0	35.7
34	13.6	32.3	17.7	32.3	34.1	36.5	10.9	31.9	31.8	35.4
35	14.5	34.0	18.8	34.5	36.6	39.1	11.8	33.7	33.9	37.7
36	14.4	36.7	19.4	36.9	38.3	40.8	11.7	36.7	35.7	39.9
37	15.2	33.9	19.2	33.9	35.7	38.4	12.4	33.2	33.6	37.3
38	3.2	32.1	10.9	30.4	30.4	36.4	−20.8	27.7	25.7	34.2
39	2.6	32.9	12.3	32.6	30.8	37.3	−24.4	29.9	25.8	35.1

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Table 11 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
40	3.2	32.4	11.2	31.0	31.1	37.4	−21.4	27.7	26.5	35.3
41	2.8	35.0	13.1	34.8	32.9	39.5	−24.9	32.1	27.6	37.5
42	3.9	33.2	11.8	31.7	31.9	38.3	−21.2	28.1	27.4	36.2
43	3.6	36.2	13.7	36.0	33.8	40.6	−24.6	33.1	28.6	38.7
44	3.9	33.3	11.6	31.7	31.9	38.4	−21.3	28.1	27.5	36.3
45	10.5	38.3	17.7	40.8	40.4	49.6	−4.6	35.3	41.3	47.2
46	−10.4	3.3	−5.0	10.3	17.0	21.6	−21.6	2.5	15.2	18.8
47	5.9	28.2	13.0	29.7	30.5	37.8	−5.0	25.3	30.9	35.5
48	11.1	43.2	19.4	46.3	44.5	55.3	−4.4	40.6	46.2	52.7
49	−9.3	12.7	−1.1	19.3	24.2	30.4	−19.7	12.2	23.1	27.6
50	4.6	29.4	13.2	31.2	31.9	39.9	−7.6	27.0	32.5	37.5
51	11.0	38.5	19.1	40.9	41.4	50.4	−2.9	35.7	42.5	47.9
52	11.9	45.8	20.7	48.9	46.5	57.9	−3.3	43.4	48.4	55.4
53	−7.7	16.4	1.2	22.6	27.2	34.1	−18.5	16.2	26.2	31.2
54	4.7	30.9	14.0	32.7	33.2	41.5	−7.3	28.5	33.8	39.2
55	12.4	40.2	20.4	42.3	41.9	51.0	−0.8	36.8	43.3	48.6
56	−11.0	28.2	4.7	29.3	22.6	30.1	−18.3	24.1	21.9	29.1
57	−14.6	31.1	3.3	32.4	24.5	33.0	−21.5	27.5	23.9	31.8
58	−11.1	28.2	4.5	29.2	22.6	30.4	−18.3	24.0	22.1	29.4
59	−11.2	32.4	4.5	32.3	24.3	32.9	−20.6	27.3	23.9	31.9
60	−10.9	28.4	4.5	29.2	22.8	30.7	−18.4	23.9	22.3	29.6
61	−14.5	34.2	3.9	35.3	26.7	35.9	−21.9	30.4	26.2	34.9
62	−10.7	28.5	4.7	29.4	22.9	30.9	−18.3	24.0	22.6	29.9
63	13.4	42.9	21.4	41.6	37.9	44.4	−12.0	41.7	35.3	44.1
64	−41.3	3.6	−24.0	9.3	13.7	18.9	−31.6	10.4	11.0	17.4
65	−40.8	−1.7	−24.7	4.7	10.0	14.8	−30.7	5.9	7.6	13.3
66	−40.5	5.1	−23.6	10.4	14.6	20.1	−31.5	11.4	12.0	18.6
67	−38.7	3.8	−23.3	9.2	12.3	17.7	−30.2	10.1	10.0	16.3
68	−40.2	−0.5	−24.2	6.0	11.0	16.2	−30.6	6.9	8.7	14.7
69	−40.5	5.8	−24.1	10.9	14.7	20.5	−32.2	11.8	12.0	18.9
70	−39.3	3.6	−23.7	9.1	12.2	17.8	−31.0	9.9	10.1	16.5
71	−39.9	0.0	−24.3	6.4	11.1	16.5	−30.8	7.1	8.9	15.0

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Table 11 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
72	−39.8	6.6	−23.5	11.6	15.4	21.2	−31.6	12.4	12.8	19.7
73	−38.7	4.2	−23.3	9.6	12.6	18.3	−30.7	10.2	10.6	17.0
74	−39.8	0.3	−24.2	6.7	11.3	16.9	−30.8	7.3	9.2	15.3
75	−18.6	−5.3	8.0	12.3	5.8	9.8	−83.4	−22.8	−15.0	−2.3
76	−16.0	−1.1	9.7	14.6	7.9	12.4	−81.4	−19.2	−13.0	1.2
77	−16.5	−1.8	7.8	12.6	6.3	10.7	−79.7	−18.6	−14.0	−0.3
78	−17.5	−4.1	8.7	13.0	6.6	10.7	−82.3	−21.7	−14.0	−1.1
79	−15.4	0.2	10.1	15.5	8.5	13.2	−81.1	−17.9	−12.6	2.3
80	−15.1	−0.2	9.1	13.9	7.6	12.0	−78.2	−17.1	−12.5	1.3
81	−17.2	−3.2	8.8	13.6	6.9	11.2	−82.0	−20.8	−13.8	−0.3
82	−14.5	1.1	11.0	16.3	9.4	14.1	−80.2	−16.9	−11.7	3.3
83	−15.0	−0.1	9.5	14.6	8.1	12.5	−79.0	−17.5	−12.2	1.9
84	−16.1	−2.2	9.7	14.5	7.8	12.2	−81.0	−19.9	−12.7	0.8
85	−8.5	8.6	−1.6	11.7	17.3	18.1	−10.0	11.2	13.2	16.1
86	−4.2	12.3	2.2	15.0	20.7	21.5	−5.1	15.0	16.6	19.5
87	1.1	13.6	5.4	15.8	24.1	25.0	−0.3	14.8	20.3	22.9
88	−4.3	11.2	2.2	14.2	20.3	21.1	−4.7	13.9	16.3	18.9
89	−7.8	9.4	−1.1	12.2	17.6	18.5	−9.5	11.6	13.5	16.6
90	−3.5	13.7	3.0	16.2	21.2	22.1	−4.2	16.1	17.1	20.1
91	−7.9	9.4	−1.3	12.2	17.5	18.5	−9.7	11.6	13.4	16.6
92	−3.3	13.8	3.1	16.3	21.3	22.2	−4.0	16.2	17.2	20.3
93	−3.6	13.0	2.6	15.5	21.2	22.1	−4.7	15.4	17.1	20.1
94	−3.4	13.0	2.8	15.6	21.4	22.2	−4.5	15.5	17.4	20.2
95	−3.8	14.2	2.1	16.4	21.1	22.0	−5.9	15.9	16.7	20.0
96	−2.4	14.9	4.1	17.4	22.3	23.3	−3.1	17.3	18.3	21.4
97	−3.6	14.7	2.3	16.8	21.4	22.4	−5.8	16.5	17.1	20.4
98	3.2	16.0	6.9	17.4	25.1	26.1	1.5	16.9	21.3	23.9
99	−1.8	14.6	3.9	16.9	21.7	22.7	−3.4	16.3	17.7	20.7
100	−2.2	14.5	3.8	16.9	22.6	23.5	−3.6	16.8	18.4	21.5
101	0.9	15.4	5.6	17.5	22.0	22.9	−0.8	16.5	18.1	21.1
102	−2.4	14.8	4.1	17.4	22.4	23.4	−3.3	17.0	18.4	21.5
103	−2.6	16.1	3.3	18.0	22.3	23.4	−4.6	17.9	18.0	21.5

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Table 11 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
104	−2.2	14.8	4.3	17.4	22.6	23.4	−3.1	17.0	18.5	21.5
105	−1.8	13.7	4.5	16.6	22.5	23.3	−2.7	16.0	18.5	21.3
106	−1.9	14.6	4.1	17.1	22.9	23.6	−3.4	16.9	18.7	21.6
107	−12.1	12.0	−0.3	17.9	20.8	25.3	−36.0	11.8	14.3	21.9
108	−15.9	2.4	−4.0	11.2	14.7	18.4	−38.4	2.5	8.7	14.9
109	−11.3	14.3	0.4	19.9	22.1	27.0	−35.8	13.6	15.6	23.8
110	−10.8	13.9	−0.1	18.4	20.0	24.6	−33.3	13.2	13.7	21.5
111	−14.1	5.9	−2.7	13.9	16.7	20.9	−37.7	5.5	10.8	17.6
112	−10.1	16.4	1.6	21.7	23.6	28.5	−35.2	15.3	17.0	25.3
113	−10.3	14.3	0.5	18.9	20.4	25.0	−33.0	13.5	14.3	22.0
114	−13.3	7.6	−1.9	15.4	18.0	22.4	−37.3	7.1	11.8	19.1
115	−9.6	16.8	2.1	22.2	24.0	28.9	−34.7	15.7	17.5	25.8
116	−9.9	14.6	0.7	19.2	20.9	25.4	−32.9	13.6	14.7	22.4
117	−13.0	8.1	−1.7	15.7	18.2	22.8	−37.1	7.4	12.1	19.5
118	−4.9	13.6	0.5	17.9	23.7	29.0	−17.6	12.6	21.8	26.0
119	−1.6	16.4	3.4	17.9	21.0	26.8	−13.9	13.3	20.4	24.0
120	−7.3	9.3	−2.3	14.6	21.2	26.3	−19.6	8.6	19.2	23.2
121	−2.8	16.3	3.4	18.2	21.6	27.2	−14.8	14.1	20.6	24.5
122	−1.9	17.5	3.0	21.2	25.9	31.9	−15.9	16.3	24.3	28.9
123	−1.9	18.0	3.5	19.9	22.3	28.5	−14.4	14.5	21.9	25.8
124	−3.9	14.9	1.3	18.9	24.8	30.3	−18.5	14.2	22.8	27.2
125	−0.1	21.3	5.8	22.4	24.7	30.7	−11.8	18.5	23.9	28.0
126	−1.6	18.2	4.1	19.6	22.4	28.4	−13.5	15.5	21.8	25.7
127	−1.8	19.1	4.1	22.8	27.8	33.9	−15.6	18.0	26.1	30.8
128	−28.0	9.3	−7.9	15.1	13.6	19.4	−32.3	9.4	11.4	17.8
129	−28.9	5.1	−9.5	11.5	10.1	15.5	−32.4	5.8	8.2	14.0
130	−26.8	10.5	−7.3	16.1	14.3	20.6	−31.4	10.4	12.2	18.9
131	−26.6	9.4	−8.2	14.8	12.8	18.8	−30.9	9.5	10.9	17.4
132	−27.9	6.4	−8.8	12.6	11.2	17.0	−31.7	6.9	9.4	15.4
133	−26.9	12.0	−7.3	17.2	15.0	21.7	−32.0	11.6	12.8	20.0
134	−26.6	9.3	−8.2	14.8	12.5	18.7	−31.0	9.4	10.9	17.4
135	−27.3	7.3	−8.6	13.3	11.4	17.7	−31.6	7.6	9.7	16.1

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Table 11 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
136	−26.3	12.6	−6.6	17.8	15.5	22.3	−31.5	12.1	13.5	20.7
137	−26.1	10.0	−7.8	15.4	13.0	19.4	−30.6	9.9	11.4	18.0
138	−26.9	8.0	−8.2	14.0	11.9	18.3	−31.4	8.2	10.2	16.8
139	−3.7	17.4	6.8	22.3	23.9	28.2	−25.5	18.6	19.6	26.5
140	−1.8	21.6	8.6	26.2	26.7	31.5	−24.5	22.1	22.3	29.9
141	−2.2	19.3	7.2	23.1	23.4	27.6	−23.2	19.8	19.3	26.1
142	−39.9	−11.6	−28.0	−2.4	10.9	13.1	−41.2	−8.0	1.0	7.7
143	−38.2	−12.5	−27.0	−3.1	10.1	12.3	−38.2	−7.7	0.1	6.5
144	−37.3	−12.8	−27.1	−3.3	10.0	12.3	−37.7	−7.8	0.4	6.6
145	−40.1	−13.3	−27.7	−3.7	9.8	12.0	−40.8	−9.4	0.8	7.0
146	−38.3	−14.1	−26.8	−4.4	9.1	11.1	−38.1	−9.1	−0.2	5.6
147	−38.9	−14.8	−27.2	−4.6	9.0	11.2	−38.3	−9.2	0.1	5.9
148	−14.5	−6.5	8.3	11.4	5.0	8.1	−64.7	−26.2	−13.9	−4.7
149	−21.5	−5.8	1.5	6.4	−2.1	2.6	−88.5	−31.8	−22.9	−8.5
150	−35.4	−11.1	−25.8	−3.1	8.7	11.8	−37.9	−6.8	0.5	6.3
151	−11.9	18.9	−11.5	19.4	21.7	27.9	−21.7	17.1	16.5	25.0
152	−11.1	3.6	−2.6	11.5	9.5	13.6	−27.2	2.5	6.9	11.4
153	2.5	22.4	5.4	22.2	18.6	24.1	−18.3	14.0	16.3	21.9
154	−16.9	−1.8	−2.9	9.9	12.4	15.7	−32.2	−0.8	6.1	11.4
155	−9.4	10.5	−0.2	16.8	17.0	21.5	−24.0	9.7	13.7	18.8
156	−1.6	19.3	7.0	22.2	20.0	24.8	−23.2	16.0	15.7	22.5
157	−5.1	16.7	1.7	19.2	20.6	25.9	−21.5	13.3	17.6	23.0
158	−14.3	−6.2	8.4	11.5	5.7	8.9	−64.6	−25.9	−13.3	−4.1
159	−14.5	−6.3	8.1	11.2	5.4	8.6	−65.0	−26.3	−13.6	−4.4
160	−34.9	−10.7	−25.5	−2.8	9.4	12.4	−37.7	−6.6	1.1	6.9
161	−8.4	23.1	−8.4	23.1	25.1	31.0	−16.4	23.0	19.5	28.3
162	−14.4	−1.7	−4.6	9.0	8.8	12.3	−26.8	−3.1	5.0	8.8
163	1.6	22.7	6.3	23.9	20.5	26.6	−19.5	17.5	19.0	25.0
164	−19.6	−4.3	−6.8	7.1	10.5	13.3	−31.4	−3.1	4.2	9.0
165	−14.3	−1.1	−3.5	9.9	10.7	14.1	−26.8	−1.1	6.3	10.2
166	−5.3	19.1	5.8	22.5	22.8	28.1	−28.2	16.2	17.6	25.4
167	−12.9	8.4	−2.2	15.8	16.8	21.6	−28.4	5.8	13.3	18.4

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Table 11 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
168	−14.1	−6.0	8.6	11.7	6.1	9.3	−64.6	−25.7	−12.9	−3.6
169	−14.2	−5.9	8.5	11.7	6.0	9.2	−65.2	−25.8	−13.1	−3.8
170	−35.8	−11.8	−26.2	−3.8	7.6	10.8	−37.9	−7.4	−0.5	5.3
171	−34.4	−3.3	−27.8	2.2	10.8	15.4	−41.3	−2.0	2.4	10.6
172	−10.3	4.4	0.8	15.5	12.1	16.6	−27.9	2.9	9.0	13.6
173	−4.0	19.5	3.2	23.1	20.0	25.9	−25.6	16.5	17.3	24.0
174	−15.3	−2.4	−4.4	9.0	10.3	13.7	−27.5	−2.0	6.0	9.8
175	−11.3	15.2	2.3	21.2	22.0	27.3	−34.0	13.9	15.9	24.1
176	−8.2	15.1	3.3	20.9	21.7	27.5	−27.3	15.8	17.9	25.2
177	−13.6	−5.5	9.0	12.1	6.6	9.8	−63.8	−25.3	−12.4	−3.1
178	−15.8	3.9	6.9	12.9	4.5	9.9	−86.4	−16.7	−16.5	0.8
179	−35.5	−11.5	−25.9	−3.6	7.9	11.1	−37.6	−7.2	−0.2	5.6
180	−35.6	−11.3	−26.2	−3.5	8.8	12.0	−38.5	−7.4	0.5	6.3
181	−8.7	11.4	1.6	20.1	16.3	22.1	−29.1	9.3	13.8	19.7
182	−7.6	13.6	2.4	21.6	17.5	23.6	−28.4	11.4	15.3	21.5
183	−18.4	−3.3	−5.7	8.1	11.6	14.4	−30.2	−2.3	5.3	10.0
184	−14.8	−2.0	−4.0	9.4	10.7	14.1	−26.9	−1.6	6.4	10.2
185	−11.7	11.7	1.7	19.7	20.5	25.5	−33.6	11.1	14.4	22.1
186	−11.7	7.6	0.4	16.8	17.7	22.7	−28.8	9.3	13.6	20.1
187	−13.9	1.4	11.6	16.5	9.1	13.6	−77.6	−20.2	−12.3	1.8
188	−33.3	0.7	−25.8	5.4	15.1	19.6	−41.0	0.1	6.2	14.3
189	−9.8	12.6	1.0	21.6	17.7	23.4	−32.0	9.1	14.2	20.4
190	−14.2	10.9	−0.1	19.4	21.4	25.9	−37.8	9.0	14.0	21.9
191	−14.0	6.9	−1.5	16.7	18.3	23.0	−33.0	6.5	12.9	19.5
192	−12.4	5.2	13.7	19.2	11.6	16.6	−79.1	−15.0	−10.3	5.4
193	−34.1	0.8	−26.9	5.7	15.3	20.1	−42.5	0.7	6.3	15.0
194	−9.3	14.6	1.8	23.8	19.2	25.5	−32.3	11.0	15.9	22.5
195	−15.2	11.4	0.3	20.3	21.8	26.7	−40.0	9.4	14.5	22.7
196	−15.0	7.3	−1.2	17.7	18.8	23.9	−35.1	7.5	13.6	20.5
197	−13.1	4.4	12.5	17.9	11.0	15.9	−81.5	−10.6	−10.6	5.4
198	−28.2	11.1	−24.2	11.3	18.6	23.5	−36.0	11.6	10.7	20.0
199	−3.2	22.8	3.0	26.1	23.5	29.8	−26.5	20.2	20.8	27.9

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Table 11 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
200	−6.0	24.6	4.8	27.0	27.5	32.9	−31.9	23.4	21.2	30.3
201	−9.1	21.4	0.9	25.2	26.1	32.1	−26.5	20.3	22.3	29.2
202	−13.2	0.2	10.9	15.5	8.2	12.4	−69.7	−22.0	−12.5	0.3
203	−38.4	−7.0	−29.7	−0.4	10.6	14.6	−43.5	−4.8	1.6	9.2
204	−14.5	3.5	−3.7	13.8	12.1	16.7	−31.3	0.4	8.1	13.2
205	−17.9	2.1	−3.3	13.0	15.5	19.3	−37.1	1.4	8.4	14.9
206	−18.3	−2.1	−4.8	10.0	12.8	16.5	−34.3	−1.1	7.5	12.8
207	−16.2	−0.7	9.2	13.9	6.6	11.0	−79.7	−15.5	−13.7	0.3
208	−27.9	7.3	−23.4	7.8	14.9	19.2	−32.6	9.5	7.4	15.6
209	−7.3	14.2	1.0	20.0	17.4	22.6	−27.8	13.3	15.0	20.8
210	−11.6	12.9	−0.1	18.0	19.4	23.8	−33.8	13.2	13.7	21.0
211	−6.4	13.9	1.8	17.9	18.9	23.3	−22.5	16.1	15.0	21.3
212	−14.8	−3.2	8.8	12.9	6.1	9.7	−70.3	−25.3	−14.5	−3.2
213	−38.6	−10.6	−30.0	−3.2	8.7	12.3	−43.2	−7.7	−0.1	6.7
214	−14.0	5.0	−1.1	16.4	13.3	18.3	−33.2	3.8	10.0	15.4
215	−21.3	−3.8	−5.8	8.9	12.3	15.9	−39.8	−3.5	5.9	11.6
216	−19.7	−1.5	−5.9	10.8	11.9	15.8	−34.7	−2.1	7.4	11.9
217	−14.8	−1.3	10.4	15.0	7.4	11.4	−75.3	−22.3	−13.7	−1.1
218	−40.3	−8.6	−31.7	−1.5	9.5	13.7	−45.8	−5.9	0.3	8.1
219	−12.6	8.7	−0.4	19.2	15.2	20.6	−33.1	7.3	11.8	17.7
220	−18.2	3.4	−4.1	14.5	16.3	20.1	−36.8	2.2	9.4	15.8
221	−20.2	3.0	−5.3	14.7	16.2	20.9	−34.6	2.8	11.6	16.9
222	−12.2	6.9	12.6	17.9	11.3	16.0	−77.9	−3.7	−10.5	6.0
223	−39.0	−7.5	−30.8	−0.8	10.4	14.7	−45.1	−5.4	1.4	9.2
224	−6.7	17.7	0.9	21.7	20.5	26.2	−28.4	16.9	17.6	24.4
225	−18.1	1.1	−4.6	11.9	14.9	18.5	−35.4	−0.5	8.0	14.0
226	−16.9	2.9	−3.4	14.3	16.4	21.0	−35.5	4.0	11.0	17.6
227	−16.3	−4.6	8.1	11.9	4.3	7.9	−75.4	−25.4	−16.1	−4.9
228	−37.7	−14.0	−29.8	−6.8	4.9	7.9	−40.8	−10.3	−2.8	2.9
229	−17.5	0.1	−6.4	10.1	8.6	12.4	−34.1	−1.7	4.4	9.4
230	−20.0	−3.8	−8.9	5.4	8.7	11.2	−31.6	−4.3	2.5	7.5
231	−19.5	−7.4	−4.8	5.8	7.4	10.8	−32.3	−4.5	3.3	7.5

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Table 11 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
232	−15.1	−3.0	9.3	13.2	5.9	9.5	−75.2	−23.5	−14.6	−3.1
233	−37.4	−7.1	−28.9	−0.6	10.3	14.3	−42.5	−4.3	2.1	9.3
234	−11.4	8.9	0.5	19.4	15.0	20.0	−32.1	7.8	11.9	17.5
235	−21.2	−0.6	−7.8	10.2	14.0	17.4	−39.0	−0.9	7.5	13.6
236	−17.9	−1.4	−5.9	9.9	10.2	14.0	−31.6	−2.8	6.1	10.1
MAXD	−41.3	45.8	−31.7	48.9	46.5	57.9	−88.5	43.4	48.4	55.4
MD	−12.8	10.9	−0.2	17.4	18.0	22.5	−31.6	7.8	11.2	18.4
MAD	15.4	13.6	9.8	17.8	18.0	22.5	32.9	15.4	15.7	18.9

Table 12: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the TPSS-D3 functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−43.4	1.1	−31.0	1.1	−1.4	5.4	−38.7	1.3	−2.5	4.5
2	−50.2	−0.2	−35.7	0.0	−2.9	4.6	−44.0	1.1	−4.1	3.6
3	−44.8	−0.2	−32.2	0.0	−1.8	5.1	−39.9	0.4	−2.8	4.2
4	−51.6	0.0	−36.9	0.2	−2.8	4.9	−45.5	1.3	−4.0	4.0
5	−48.2	0.1	−34.9	0.0	−2.2	5.2	−43.1	0.6	−3.5	4.2
6	−52.1	0.1	−37.4	0.3	−2.8	5.0	−46.2	1.3	−4.1	4.1
7	−48.0	0.2	−34.8	0.1	−1.9	5.4	−43.1	0.6	−3.1	4.3
8	−23.6	−5.6	−1.7	3.8	−5.1	0.1	−91.1	−24.6	−25.4	−8.9
9	−23.7	−4.5	−1.3	4.5	−4.3	1.1	−93.3	−21.8	−25.0	−7.6
10	−25.8	−13.1	0.2	4.5	−2.4	1.8	−85.0	−29.5	−22.8	−9.9
11	−24.5	−11.0	0.6	5.0	−1.5	2.7	−85.2	−26.5	−22.1	−8.7
12	−23.4	−5.2	−1.5	4.0	−4.6	0.7	−91.4	−24.3	−24.9	−8.3
13	−22.4	−3.0	0.0	6.0	−3.0	2.7	−92.3	−20.5	−23.6	−6.0
14	−25.7	−12.8	0.2	4.7	−2.4	1.9	−85.1	−29.4	−22.6	−9.7
15	−24.4	−8.8	0.9	5.8	−1.0	3.6	−87.6	−22.6	−22.0	−7.0
16	−22.4	−2.5	−0.6	5.3	−3.3	2.4	−92.2	−21.1	−24.0	−6.3
17	−22.2	−2.6	0.2	6.5	−2.6	3.0	−92.3	−20.2	−23.3	−5.5

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Table 12 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
18	−25.5	−12.2	0.4	5.3	−2.1	2.3	−85.2	−28.7	−22.6	−8.9
19	−24.5	−8.2	0.8	6.0	−1.2	3.6	−88.3	−21.6	−22.2	−6.5
20	−22.2	−2.2	−0.5	5.6	−3.1	2.6	−92.4	−20.9	−23.8	−6.0
21	−15.5	3.1	−11.0	3.5	5.3	7.7	−18.1	3.3	3.0	6.5
22	−21.8	−8.8	−14.7	−2.9	1.7	3.1	−21.5	−4.5	−1.0	1.4
23	−16.5	2.5	−12.2	3.1	5.3	7.7	−19.0	2.4	2.5	6.2
24	−17.3	1.7	−12.7	2.5	4.4	6.4	−20.0	1.8	1.7	5.2
25	−18.2	1.8	−13.4	2.4	4.2	6.5	−21.1	1.8	1.5	5.3
26	−16.2	2.1	−11.8	2.7	4.8	7.0	−18.8	1.9	2.3	5.8
27	−15.8	2.7	−11.5	3.0	5.2	7.6	−18.7	2.5	2.8	6.3
28	−14.2	4.5	−9.9	4.6	6.3	8.8	−16.7	4.4	4.1	7.7
29	−16.7	2.6	−12.3	3.1	5.3	7.7	−19.1	2.5	2.6	6.3
30	−18.9	2.4	−13.9	2.5	4.1	6.6	−21.2	2.1	1.6	5.5
31	−21.0	−4.4	−14.4	−0.5	3.8	5.5	−21.1	−0.9	0.6	3.7
32	−18.7	3.1	−13.7	3.4	4.9	7.4	−21.4	3.1	2.3	6.4
33	−14.9	3.8	−10.9	3.8	5.6	8.3	−17.7	3.2	3.5	7.2
34	−13.6	5.1	−9.5	5.1	6.9	9.3	−16.3	4.7	4.6	8.2
35	−15.8	3.7	−11.5	4.2	6.3	8.8	−18.4	3.4	3.6	7.4
36	−17.4	4.9	−12.3	5.1	6.5	9.1	−20.1	4.9	3.9	8.2
37	−13.6	5.1	−9.6	5.1	6.9	9.6	−16.4	4.4	4.8	8.5
38	−27.5	1.4	−19.8	−0.2	−0.3	5.7	−51.5	−3.0	−5.0	3.6
39	−30.8	−0.5	−21.1	−0.8	−2.5	3.9	−57.8	−3.5	−7.6	1.7
40	−28.1	1.2	−20.1	−0.3	−0.1	6.2	−52.6	−3.5	−4.7	4.1
41	−32.3	−0.2	−22.1	−0.4	−2.3	4.3	−60.1	−3.1	−7.6	2.3
42	−27.7	1.6	−19.8	0.1	0.3	6.7	−52.8	−3.5	−4.2	4.6
43	−32.7	0.0	−22.5	−0.3	−2.4	4.4	−60.8	−3.1	−7.7	2.5
44	−27.8	1.6	−20.0	0.0	0.2	6.7	−53.0	−3.6	−4.2	4.6
45	−35.6	−7.9	−28.4	−5.4	−5.8	3.5	−50.7	−10.9	−4.9	1.0
46	−35.2	−21.5	−29.8	−14.5	−7.8	−3.1	−46.4	−22.2	−9.5	−5.9
47	−27.5	−5.2	−20.4	−3.7	−3.0	4.3	−38.4	−8.2	−2.6	2.0
48	−41.5	−9.4	−33.3	−6.3	−8.1	2.6	−57.1	−12.0	−6.5	0.0
49	−42.6	−20.7	−34.4	−14.1	−9.2	−2.9	−53.1	−21.2	−10.3	−5.7

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Table 12 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
50	−31.5	−6.7	−22.8	−4.8	−4.2	3.8	−43.6	−9.1	−3.6	1.4
51	−34.4	−7.0	−26.4	−4.5	−4.1	5.0	−48.3	−9.8	−2.9	2.5
52	−43.7	−9.7	−34.9	−6.7	−9.0	2.4	−58.9	−12.1	−7.1	−0.2
53	−44.4	−20.4	−35.6	−14.2	−9.5	−2.7	−55.3	−20.6	−10.5	−5.6
54	−33.0	−6.9	−23.7	−5.1	−4.5	3.7	−45.1	−9.2	−4.0	1.4
55	−33.3	−5.5	−25.4	−3.5	−3.8	5.3	−46.5	−8.9	−2.5	2.9
56	−37.4	1.8	−21.7	2.9	−3.8	3.6	−44.7	−2.4	−4.5	2.7
57	−44.7	1.0	−26.8	2.3	−5.6	2.9	−51.6	−2.6	−6.1	1.8
58	−37.7	1.6	−22.2	2.5	−4.1	3.8	−45.0	−2.7	−4.5	2.8
59	−41.1	2.6	−25.3	2.5	−5.6	3.1	−50.5	−2.6	−5.9	2.1
60	−37.6	1.6	−22.3	2.5	−4.0	4.0	−45.1	−2.8	−4.4	2.9
61	−47.4	1.2	−29.0	2.3	−6.2	3.0	−54.9	−2.6	−6.7	2.0
62	−37.6	1.7	−22.1	2.5	−3.9	4.0	−45.1	−2.9	−4.3	3.0
63	−24.3	5.2	−16.3	3.9	0.3	6.7	−49.7	4.0	−2.4	6.5
64	−62.0	−17.1	−44.7	−11.4	−7.0	−1.8	−52.3	−10.3	−9.7	−3.3
65	−58.6	−19.6	−42.6	−13.1	−7.9	−3.0	−48.6	−12.0	−10.3	−4.6
66	−62.1	−16.5	−45.2	−11.2	−7.0	−1.5	−53.2	−10.2	−9.6	−3.0
67	−57.8	−15.4	−42.4	−10.0	−6.9	−1.5	−49.4	−9.1	−9.2	−2.9
68	−58.8	−19.0	−42.8	−12.5	−7.6	−2.3	−49.1	−11.6	−9.8	−3.9
69	−62.9	−16.5	−46.5	−11.5	−7.7	−1.9	−54.5	−10.6	−10.4	−3.5
70	−58.9	−15.9	−43.2	−10.5	−7.4	−1.8	−50.5	−9.7	−9.4	−3.1
71	−59.0	−19.1	−43.4	−12.7	−8.0	−2.6	−49.9	−12.1	−10.2	−4.2
72	−62.4	−16.0	−46.0	−10.9	−7.2	−1.4	−54.2	−10.1	−9.8	−2.9
73	−58.6	−15.7	−43.2	−10.3	−7.3	−1.6	−50.6	−9.7	−9.3	−2.9
74	−59.1	−19.0	−43.5	−12.6	−8.0	−2.4	−50.1	−12.0	−10.1	−4.0
75	−28.1	−14.8	−1.4	2.8	−3.7	0.3	−92.8	−32.3	−24.5	−11.7
76	−27.3	−12.5	−1.6	3.2	−3.5	1.1	−92.7	−30.6	−24.4	−10.2
77	−27.2	−12.4	−2.9	1.9	−4.4	0.0	−90.4	−29.3	−24.7	−10.9
78	−27.5	−14.0	−1.3	3.0	−3.3	0.7	−92.2	−31.7	−23.9	−11.1
79	−27.3	−11.7	−1.7	3.6	−3.4	1.3	−93.0	−29.8	−24.5	−9.6
80	−26.1	−11.3	−1.9	2.9	−3.4	1.0	−89.2	−28.1	−23.5	−9.7
81	−27.5	−13.6	−1.6	3.2	−3.5	0.8	−92.4	−31.2	−24.1	−10.7

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Table 12 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
82	−26.5	−10.8	−1.0	4.3	−2.6	2.2	−92.2	−28.9	−23.7	−8.7
83	−26.3	−11.3	−1.8	3.4	−3.2	1.3	−90.2	−28.8	−23.5	−9.4
84	−26.6	−12.6	−0.7	4.0	−2.6	1.7	−91.5	−30.3	−23.2	−9.7
85	−28.6	−11.5	−21.6	−8.4	−2.7	−2.0	−30.0	−8.9	−6.9	−3.9
86	−26.3	−9.8	−19.9	−7.1	−1.4	−0.6	−27.2	−7.1	−5.5	−2.6
87	−18.3	−5.8	−14.0	−3.6	4.7	5.5	−19.8	−4.6	0.9	3.4
88	−25.7	−10.2	−19.2	−7.2	−1.1	−0.4	−26.2	−7.5	−5.1	−2.5
89	−28.4	−11.2	−21.7	−8.4	−3.0	−2.1	−30.1	−9.0	−7.1	−4.1
90	−26.3	−9.1	−19.9	−6.7	−1.7	−0.7	−27.0	−6.7	−5.8	−2.7
91	−28.6	−11.3	−21.9	−8.5	−3.2	−2.2	−30.3	−9.0	−7.2	−4.1
92	−26.2	−9.0	−19.7	−6.5	−1.5	−0.6	−26.8	−6.6	−5.6	−2.6
93	−26.2	−9.7	−20.0	−7.1	−1.4	−0.6	−27.3	−7.2	−5.5	−2.6
94	−26.0	−9.6	−19.8	−7.0	−1.2	−0.5	−27.2	−7.1	−5.3	−2.5
95	−25.8	−7.7	−19.8	−5.6	−0.9	0.0	−27.9	−6.0	−5.2	−1.9
96	−25.5	−8.2	−18.9	−5.6	−0.8	0.2	−26.1	−5.8	−4.8	−1.7
97	−25.6	−7.3	−19.7	−5.2	−0.6	0.4	−27.8	−5.5	−5.0	−1.6
98	−16.8	−3.9	−13.1	−2.6	5.1	6.1	−18.5	−3.1	1.3	4.0
99	−24.4	−8.0	−18.7	−5.7	−0.9	0.1	−26.0	−6.3	−4.9	−1.9
100	−25.2	−8.5	−19.1	−6.0	−0.3	0.5	−26.6	−6.2	−4.5	−1.5
101	−22.2	−7.8	−17.6	−5.7	−1.1	−0.2	−24.0	−6.7	−5.0	−2.1
102	−25.5	−8.3	−19.0	−5.8	−0.7	0.2	−26.4	−6.1	−4.7	−1.7
103	−25.4	−6.6	−19.4	−4.8	−0.5	0.7	−27.3	−4.9	−4.8	−1.2
104	−25.4	−8.3	−18.9	−5.8	−0.5	0.3	−26.3	−6.1	−4.6	−1.7
105	−24.7	−9.2	−18.5	−6.3	−0.4	0.4	−25.7	−7.0	−4.4	−1.6
106	−25.0	−8.4	−18.9	−6.0	−0.1	0.6	−26.4	−6.2	−4.3	−1.4
107	−38.6	−14.6	−26.9	−8.7	−5.8	−1.3	−62.6	−14.8	−12.3	−4.7
108	−36.5	−18.3	−24.7	−9.4	−5.9	−2.2	−59.1	−18.2	−11.9	−5.8
109	−39.7	−14.1	−27.9	−8.4	−6.2	−1.3	−64.1	−14.8	−12.7	−4.6
110	−36.5	−11.9	−25.8	−7.3	−5.7	−1.1	−59.1	−12.6	−12.1	−4.3
111	−36.9	−17.0	−25.5	−8.9	−6.1	−1.9	−60.5	−17.3	−12.0	−5.3
112	−39.7	−13.2	−28.0	−7.8	−6.0	−1.1	−64.8	−14.3	−12.6	−4.3
113	−36.5	−11.9	−25.7	−7.3	−5.7	−1.1	−59.1	−12.7	−11.8	−4.2

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Table 12 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
114	−37.2	−16.3	−25.8	−8.5	−6.0	−1.5	−61.2	−16.9	−12.1	−4.8
115	−39.3	−12.9	−27.6	−7.5	−5.7	−0.8	−64.5	−14.1	−12.3	−3.9
116	−36.6	−12.1	−26.0	−7.5	−5.8	−1.3	−59.6	−13.1	−12.0	−4.3
117	−37.2	−16.1	−25.9	−8.4	−6.0	−1.4	−61.3	−16.8	−12.0	−4.7
118	−37.9	−19.4	−32.5	−15.1	−9.3	−4.1	−50.6	−20.5	−11.3	−7.1
119	−30.1	−12.1	−25.2	−10.6	−7.5	−1.8	−42.5	−15.3	−8.2	−4.5
120	−38.0	−21.4	−32.9	−16.0	−9.5	−4.3	−50.2	−22.0	−11.5	−7.5
121	−31.7	−12.6	−25.6	−10.7	−7.4	−1.8	−43.7	−14.8	−8.3	−4.4
122	−36.5	−17.1	−31.6	−13.4	−8.7	−2.7	−50.5	−18.3	−10.3	−5.7
123	−32.4	−12.5	−27.0	−10.6	−8.1	−1.9	−44.8	−15.9	−8.6	−4.7
124	−38.1	−19.2	−32.9	−15.3	−9.3	−3.8	−52.6	−19.9	−11.4	−7.0
125	−31.8	−10.4	−25.9	−9.3	−7.0	−1.0	−43.5	−13.2	−7.8	−3.7
126	−31.3	−11.5	−25.6	−10.1	−7.3	−1.3	−43.1	−14.2	−7.9	−4.0
127	−38.4	−17.5	−32.5	−13.8	−8.8	−2.7	−52.2	−18.6	−10.5	−5.8
128	−50.9	−13.6	−30.8	−7.8	−9.3	−3.5	−55.2	−13.5	−11.6	−5.1
129	−49.0	−15.0	−29.6	−8.6	−10.0	−4.6	−52.5	−14.3	−11.9	−6.1
130	−50.0	−12.8	−30.6	−7.2	−9.0	−2.6	−54.7	−12.8	−11.1	−4.3
131	−48.1	−12.1	−29.8	−6.7	−8.8	−2.8	−52.4	−12.0	−10.7	−4.2
132	−48.8	−14.5	−29.7	−8.3	−9.8	−4.0	−52.6	−14.0	−11.6	−5.6
133	−52.0	−13.1	−32.4	−7.9	−10.1	−3.4	−57.1	−13.5	−12.3	−5.1
134	−48.4	−12.5	−30.0	−7.0	−9.3	−3.1	−52.8	−12.4	−10.9	−4.4
135	−49.1	−14.5	−30.4	−8.4	−10.3	−4.1	−53.4	−14.2	−12.0	−5.6
136	−51.5	−12.7	−31.9	−7.5	−9.7	−3.0	−56.8	−13.2	−11.7	−4.6
137	−48.5	−12.4	−30.2	−7.0	−9.4	−3.0	−53.0	−12.5	−11.0	−4.4
138	−49.0	−14.1	−30.3	−8.1	−10.2	−3.8	−53.5	−13.9	−11.9	−5.3
139	−31.0	−9.9	−20.5	−4.9	−3.4	0.9	−52.8	−8.7	−7.7	−0.8
140	−32.2	−8.7	−21.8	−4.2	−3.7	1.1	−54.9	−8.3	−8.1	−0.5
141	−29.2	−7.6	−19.8	−3.9	−3.6	0.6	−50.2	−7.2	−7.6	−0.9
142	−55.1	−26.7	−43.2	−17.6	−4.3	−2.1	−56.4	−23.2	−14.2	−7.5
143	−52.0	−26.2	−40.7	−16.9	−3.6	−1.5	−51.9	−21.4	−13.6	−7.3
144	−51.4	−26.9	−41.2	−17.5	−4.1	−1.8	−51.8	−21.9	−13.7	−7.5
145	−55.1	−28.4	−42.8	−18.7	−5.3	−3.1	−55.9	−24.5	−14.3	−8.1

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Table 12 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
146	−51.9	−27.7	−40.4	−18.0	−4.5	−2.5	−51.7	−22.7	−13.8	−8.0
147	−52.9	−28.9	−41.2	−18.6	−5.0	−2.8	−52.3	−23.3	−13.9	−8.1
148	−19.5	−11.5	3.3	6.4	0.0	3.1	−69.7	−31.2	−18.9	−9.7
149	−31.4	−15.7	−8.4	−3.4	−12.0	−7.3	−98.3	−41.7	−32.8	−18.3
150	−44.8	−20.5	−35.2	−12.5	−0.7	2.4	−47.4	−16.2	−8.9	−3.1
151	−33.8	−3.0	−33.4	−2.5	−0.2	6.0	−43.5	−4.8	−5.4	3.1
152	−25.9	−11.2	−17.4	−3.3	−5.3	−1.2	−42.0	−12.3	−7.9	−3.4
153	−20.6	−0.6	−17.7	−0.9	−4.5	1.0	−41.4	−9.0	−6.8	−1.2
154	−31.5	−16.4	−17.5	−4.7	−2.3	1.1	−46.8	−15.5	−8.5	−3.3
155	−30.9	−10.9	−21.6	−4.7	−4.5	0.0	−45.5	−11.8	−7.7	−2.7
156	−24.5	−3.7	−16.0	−0.7	−2.9	1.9	−46.2	−6.9	−7.2	−0.4
157	−29.2	−7.4	−22.4	−4.8	−3.4	1.8	−45.6	−10.8	−6.4	−1.1
158	−19.4	−11.3	3.3	6.4	0.6	3.8	−69.7	−31.0	−18.3	−9.1
159	−19.6	−11.4	3.0	6.2	0.3	3.5	−70.1	−31.4	−18.7	−9.5
160	−44.4	−20.1	−35.0	−12.3	−0.1	3.0	−47.2	−16.1	−8.4	−2.6
161	−30.8	0.7	−30.8	0.7	2.7	8.6	−38.7	0.6	−2.9	6.0
162	−26.9	−14.2	−17.1	−3.5	−3.7	−0.2	−39.3	−15.6	−7.5	−3.8
163	−23.2	−2.1	−18.5	−0.9	−4.3	1.9	−44.3	−7.3	−5.8	0.2
164	−32.4	−17.2	−19.6	−5.7	−2.3	0.4	−44.3	−15.9	−8.7	−3.8
165	−29.6	−16.4	−18.8	−5.4	−4.6	−1.2	−42.1	−16.4	−9.0	−5.1
166	−30.8	−6.4	−19.7	−3.0	−2.6	2.6	−53.6	−9.3	−7.9	−0.1
167	−35.5	−14.1	−24.7	−6.8	−5.7	−0.9	−50.9	−16.8	−9.3	−4.2
168	−19.3	−11.1	3.4	6.6	1.0	4.2	−69.7	−30.8	−18.0	−8.8
169	−19.5	−11.2	3.2	6.4	0.7	3.9	−70.5	−31.1	−18.4	−9.1
170	−45.2	−21.2	−35.6	−13.3	−1.8	1.4	−47.4	−16.9	−9.9	−4.2
171	−49.8	−18.7	−43.2	−13.2	−4.6	0.0	−56.7	−17.4	−13.0	−4.8
172	−27.4	−12.7	−16.3	−1.6	−5.0	−0.5	−45.0	−14.2	−8.1	−3.5
173	−29.9	−6.5	−22.7	−2.8	−5.9	0.0	−51.5	−9.5	−8.6	−1.9
174	−29.9	−17.0	−19.0	−5.6	−4.3	−0.9	−42.1	−16.6	−8.6	−4.8
175	−36.8	−10.3	−23.2	−4.3	−3.5	1.8	−59.5	−11.6	−9.6	−1.4
176	−35.2	−11.8	−23.6	−6.0	−5.3	0.6	−54.2	−11.1	−9.0	−1.7
177	−18.8	−10.7	3.9	7.0	1.4	4.7	−68.9	−30.4	−17.5	−8.3

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Table 12 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
178	−28.9	−9.2	−6.3	−0.3	−8.6	−3.2	−99.5	−29.8	−29.6	−12.3
179	−44.9	−20.9	−35.3	−13.0	−1.5	1.7	−47.1	−16.6	−9.6	−3.9
180	−45.2	−21.0	−35.9	−13.2	−0.9	2.3	−48.1	−17.0	−9.2	−3.3
181	−31.7	−11.6	−21.4	−2.9	−6.6	−0.9	−52.1	−13.7	−9.2	−3.3
182	−31.7	−10.6	−21.7	−2.5	−6.6	−0.6	−52.5	−12.7	−8.8	−2.6
183	−31.3	−16.1	−18.5	−4.7	−1.3	1.5	−43.1	−15.1	−7.6	−2.8
184	−29.3	−16.5	−18.5	−5.1	−3.8	−0.4	−41.4	−16.1	−8.1	−4.3
185	−35.6	−12.1	−22.1	−4.1	−3.3	1.6	−57.5	−12.8	−9.4	−1.7
186	−34.6	−15.2	−22.5	−6.0	−5.1	−0.1	−51.7	−13.5	−9.3	−2.8
187	−24.4	−9.2	1.1	5.9	−1.5	3.0	−88.2	−30.8	−22.9	−8.8
188	−51.5	−17.5	−44.1	−12.9	−3.1	1.4	−59.3	−18.1	−12.0	−3.9
189	−36.3	−13.8	−25.5	−4.8	−8.7	−3.1	−58.4	−17.3	−12.3	−6.1
190	−41.4	−16.3	−27.3	−7.8	−5.9	−1.3	−65.0	−18.2	−13.2	−5.4
191	−39.9	−19.0	−27.4	−9.2	−7.6	−2.9	−58.9	−19.4	−13.0	−6.4
192	−24.8	−7.2	1.3	6.9	−0.8	4.3	−91.5	−27.4	−22.6	−7.0
193	−52.8	−17.9	−45.6	−12.9	−3.4	1.4	−61.2	−18.0	−12.3	−3.7
194	−37.7	−13.9	−26.6	−4.7	−9.3	−3.0	−60.8	−17.5	−12.6	−6.0
195	−43.9	−17.3	−28.4	−8.4	−6.9	−2.0	−68.7	−19.3	−14.2	−6.0
196	−42.8	−20.5	−29.1	−10.1	−9.0	−3.9	−62.9	−20.3	−14.3	−7.3
197	−26.3	−8.8	−0.6	4.7	−2.2	2.7	−94.6	−23.8	−23.8	−7.8
198	−49.4	−10.1	−45.4	−10.0	−2.6	2.3	−57.2	−9.7	−10.6	−1.2
199	−33.8	−7.7	−27.5	−4.4	−7.1	−0.8	−57.1	−10.4	−9.8	−2.6
200	−39.1	−8.4	−28.3	−6.0	−5.5	−0.1	−64.9	−9.7	−11.8	−2.8
201	−42.5	−12.0	−32.5	−8.2	−7.3	−1.4	−59.9	−13.1	−11.2	−4.2
202	−22.3	−8.8	1.8	6.5	−0.9	3.3	−78.8	−31.1	−21.6	−8.8
203	−53.6	−22.2	−44.9	−15.6	−4.6	−0.6	−58.7	−20.0	−13.6	−6.0
204	−34.5	−16.5	−23.6	−6.2	−7.9	−3.3	−51.3	−19.5	−11.8	−6.7
205	−39.4	−19.4	−24.8	−8.5	−6.0	−2.2	−58.6	−20.1	−13.1	−6.6
206	−38.8	−22.6	−25.4	−10.5	−7.8	−4.1	−54.8	−21.7	−13.1	−7.7
207	−27.1	−11.7	−1.7	3.0	−4.3	0.1	−90.6	−26.5	−24.7	−10.6
208	−45.8	−10.7	−41.3	−10.1	−3.1	1.3	−50.6	−8.5	−10.6	−2.4
209	−33.1	−11.6	−24.8	−5.8	−8.4	−3.2	−53.6	−12.5	−10.8	−5.0

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Table 12 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
210	−37.6	−13.1	−26.1	−8.0	−6.7	−2.2	−59.8	−12.8	−12.4	−5.0
211	−31.6	−11.3	−23.4	−7.3	−6.3	−1.8	−47.6	−9.1	−10.1	−3.8
212	−22.3	−10.7	1.3	5.4	−1.4	2.2	−77.8	−32.8	−22.0	−10.7
213	−51.0	−23.1	−42.4	−15.6	−3.8	−0.1	−55.6	−20.2	−12.5	−5.7
214	−35.6	−16.7	−22.8	−5.2	−8.4	−3.4	−54.9	−17.9	−11.7	−6.3
215	−38.6	−21.2	−23.1	−8.5	−5.1	−1.5	−57.2	−20.9	−11.4	−5.7
216	−40.2	−22.0	−26.4	−9.7	−8.6	−4.7	−55.2	−22.6	−13.0	−8.6
217	−23.9	−10.4	1.3	5.8	−1.8	2.3	−84.4	−31.4	−22.8	−10.3
218	−54.9	−23.3	−46.3	−16.2	−5.2	−1.0	−60.5	−20.5	−14.3	−6.6
219	−37.4	−16.1	−25.1	−5.6	−9.6	−4.2	−57.9	−17.5	−12.9	−7.0
220	−41.4	−19.8	−27.2	−8.6	−6.8	−3.1	−59.9	−20.9	−13.7	−7.3
221	−44.3	−21.2	−29.4	−9.4	−7.9	−3.2	−58.7	−21.4	−12.5	−7.2
222	−25.8	−6.7	−1.1	4.3	−2.4	2.4	−91.5	−17.3	−24.1	−7.6
223	−53.8	−22.3	−45.6	−15.6	−4.4	−0.1	−59.9	−20.2	−13.4	−5.6
224	−35.0	−10.6	−27.4	−6.6	−7.8	−2.1	−56.7	−11.4	−10.7	−3.9
225	−37.5	−18.3	−24.0	−7.5	−4.5	−0.9	−54.8	−19.9	−11.4	−5.4
226	−41.4	−21.6	−27.9	−10.3	−8.2	−3.5	−60.0	−20.6	−13.6	−7.0
227	−23.7	−12.0	0.7	4.6	−3.0	0.5	−82.8	−32.8	−23.5	−12.3
228	−47.1	−23.4	−39.1	−16.2	−4.5	−1.5	−50.1	−19.7	−12.1	−6.4
229	−34.5	−17.0	−23.5	−6.9	−8.4	−4.6	−51.2	−18.7	−12.7	−7.6
230	−32.5	−16.3	−21.4	−7.1	−3.8	−1.3	−44.1	−16.8	−10.1	−5.0
231	−34.1	−21.9	−19.3	−8.7	−7.1	−3.7	−46.8	−19.0	−11.3	−7.0
232	−23.0	−11.0	1.3	5.2	−2.1	1.5	−83.1	−31.5	−22.5	−11.0
233	−51.5	−21.3	−43.1	−14.7	−3.9	0.1	−56.6	−18.4	−12.0	−4.9
234	−34.7	−14.4	−22.8	−3.9	−8.2	−3.2	−55.3	−15.4	−11.4	−5.7
235	−40.5	−19.9	−27.0	−9.0	−5.2	−1.9	−58.2	−20.1	−11.7	−5.7
236	−36.1	−19.5	−24.1	−8.3	−8.0	−4.1	−49.8	−21.0	−12.1	−8.1
MAXD	−62.9	−28.9	−46.5	−18.7	−12.0	9.6	−99.5	−41.7	−32.8	−18.3
MD	−34.5	−10.9	−22.0	−4.4	−3.8	0.8	−53.4	−14.0	−10.5	−3.3
MAD	34.5	11.5	22.3	6.7	4.7	2.7	53.4	14.4	11.0	5.1

Table 13: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the XLYP functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−28.5	26.4	−10.9	28.6	29.0	34.7	−23.2	26.6	23.9	32.7
2	−34.2	27.6	−13.9	29.9	30.1	36.4	−27.1	28.8	24.7	34.4
3	−30.5	24.7	−12.9	26.7	28.0	33.8	−24.9	25.3	22.9	31.7
4	−34.9	28.9	−14.4	31.1	31.2	37.6	−28.0	30.1	25.7	35.8
5	−32.6	27.1	−13.9	29.0	29.9	36.1	−26.9	27.6	24.3	34.0
6	−35.0	29.5	−14.6	31.7	31.7	38.2	−28.4	30.6	26.1	36.4
7	−32.3	27.4	−13.7	29.2	30.3	36.3	−26.8	27.7	24.8	34.2
8	−10.9	14.6	17.8	25.5	19.3	23.9	−91.4	−6.4	−12.7	10.7
9	−10.1	17.1	19.2	27.4	21.3	26.1	−92.9	−1.6	−11.4	13.3
10	−18.6	−0.4	13.4	19.3	16.1	19.8	−89.6	−18.1	−15.3	3.3
11	−16.3	2.8	14.5	20.7	17.8	21.5	−89.7	−14.3	−13.8	5.5
12	−10.1	15.6	18.3	26.2	20.3	25.0	−91.1	−5.3	−11.8	11.8
13	−8.1	19.4	20.9	29.4	23.1	28.2	−91.4	0.4	−9.5	15.5
14	−18.0	0.3	13.6	19.7	16.4	20.2	−89.4	−17.7	−14.9	3.8
15	−13.8	8.3	17.5	24.4	21.0	25.1	−90.3	−7.0	−11.3	10.1
16	−7.1	21.0	21.7	30.1	23.9	28.9	−90.7	0.1	−8.9	16.3
17	−7.6	20.1	21.5	30.2	23.8	28.8	−91.0	1.1	−9.0	16.3
18	−17.3	1.7	14.5	21.1	17.4	21.3	−88.9	−16.1	−14.2	5.5
19	−12.9	10.2	18.4	25.7	21.9	26.2	−90.3	−4.8	−10.6	11.8
20	−6.6	21.6	22.2	30.8	24.5	29.5	−90.6	0.7	−8.4	16.9
21	10.8	36.7	19.0	38.2	42.6	44.4	5.6	35.8	36.7	41.4
22	−7.9	10.5	2.0	17.5	26.1	27.1	−9.8	14.2	20.5	23.7
23	12.2	38.8	20.7	40.6	45.7	47.4	7.7	37.6	39.3	44.2
24	9.7	36.4	18.2	38.2	42.9	44.3	4.6	35.4	36.5	41.3
25	9.5	37.5	18.4	39.1	43.6	45.3	4.2	36.2	37.3	42.4
26	10.0	35.6	18.0	37.0	42.0	43.7	5.1	34.3	36.0	40.6
27	10.6	36.6	18.6	37.7	42.5	44.2	5.3	35.2	36.5	41.2
28	13.0	39.0	20.8	40.0	44.3	46.1	7.9	37.6	38.4	43.2
29	13.0	39.8	21.3	41.4	46.4	48.1	8.4	38.4	40.1	45.0

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Table 13 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
30	12.5	42.1	21.8	43.1	47.3	49.1	7.8	40.5	41.0	46.2
31	0.7	24.0	10.7	28.9	36.8	38.0	−2.1	26.6	30.4	34.5
32	11.5	41.9	20.8	43.1	47.2	49.0	6.5	40.6	40.7	46.2
33	14.7	40.8	22.4	41.6	46.0	48.0	9.6	38.9	40.2	45.1
34	14.0	40.0	21.6	40.7	45.0	46.8	8.6	38.2	39.1	43.9
35	14.4	41.5	22.8	43.1	48.1	49.8	9.7	40.0	41.7	46.8
36	14.2	45.1	23.4	46.2	50.1	52.0	8.9	43.8	43.6	49.3
37	16.5	42.5	24.1	43.2	47.6	49.7	11.3	40.5	41.9	46.8
38	3.7	41.2	16.3	40.8	41.9	46.7	−26.7	35.3	31.2	42.3
39	3.9	43.2	19.1	44.2	44.1	49.3	−30.3	38.7	32.7	44.8
40	4.0	41.9	16.7	41.5	42.8	47.9	−27.0	35.7	32.2	43.5
41	4.4	46.2	20.1	47.0	46.7	52.1	−30.9	41.6	34.9	47.6
42	4.8	42.7	17.3	42.2	43.6	48.8	−26.7	36.2	33.0	44.4
43	5.3	47.8	21.0	48.5	48.0	53.6	−30.4	43.0	36.1	49.1
44	4.7	42.9	17.2	42.2	43.7	48.9	−26.8	36.2	33.1	44.5
45	10.0	46.1	21.8	49.2	52.1	59.5	−12.4	39.9	47.7	55.3
46	−11.7	5.5	−4.0	13.2	23.4	27.1	−29.2	3.6	18.2	22.8
47	0.6	30.7	12.0	32.9	37.3	43.0	−15.9	25.5	33.4	39.2
48	9.8	51.3	23.3	55.3	57.2	65.7	−13.2	45.5	53.3	61.6
49	−11.8	16.0	−0.1	23.5	32.4	37.4	−28.7	13.9	27.3	33.0
50	−1.0	32.6	12.5	34.9	39.4	45.7	−19.1	27.9	35.4	41.8
51	9.1	45.1	21.4	47.8	51.6	58.7	−11.8	39.4	47.3	54.3
52	10.9	54.6	25.1	58.5	59.9	68.9	−11.9	49.0	56.0	64.9
53	−10.5	20.2	2.0	27.1	35.8	41.2	−28.4	18.3	30.5	36.8
54	−1.1	34.3	13.2	36.5	40.9	47.5	−19.2	29.6	36.8	43.6
55	10.1	46.7	22.6	49.0	51.8	59.0	−9.6	40.4	48.0	54.8
56	−19.4	30.0	1.8	32.9	29.4	35.6	−30.3	24.5	23.6	32.8
57	−24.3	33.0	−0.4	36.3	31.8	38.9	−35.1	28.1	26.0	36.1
58	−19.4	30.0	1.4	32.6	29.2	35.8	−30.3	24.4	23.7	33.0
59	−21.6	33.3	−0.4	34.9	30.0	37.2	−35.2	26.9	24.5	34.7
60	−19.2	30.2	1.3	32.6	29.3	36.0	−30.4	24.3	23.8	33.2
61	−24.6	36.3	−0.2	39.4	34.3	42.1	−36.1	31.3	28.3	39.5

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Table 13 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
62	−19.1	30.3	1.4	32.7	29.4	36.1	−30.4	24.4	24.0	33.3
63	15.9	54.5	29.1	53.9	51.4	56.6	−17.0	51.4	42.8	54.3
64	−52.2	3.9	−30.0	11.3	19.4	23.7	−41.4	11.1	13.0	21.0
65	−50.5	−1.8	−30.2	6.3	15.2	19.2	−39.1	6.5	9.3	16.5
66	−51.3	5.6	−29.8	12.4	20.3	24.9	−41.4	12.3	13.9	22.2
67	−49.3	3.7	−29.8	10.5	17.1	21.6	−40.3	10.4	11.4	19.3
68	−49.9	−0.3	−30.0	7.5	16.1	20.5	−39.2	7.6	10.3	17.8
69	−51.4	6.3	−30.5	12.9	20.3	25.2	−42.2	12.7	13.9	22.5
70	−50.1	3.6	−30.4	10.3	17.0	21.7	−41.2	10.2	11.4	19.5
71	−49.7	0.0	−30.3	7.6	16.0	20.6	−39.6	7.6	10.2	17.9
72	−50.8	7.0	−30.0	13.5	21.0	25.8	−41.7	13.2	14.5	23.2
73	−49.4	4.1	−30.0	10.8	17.4	22.2	−40.9	10.5	11.9	20.0
74	−49.6	0.4	−30.3	7.9	16.2	20.9	−39.7	7.8	10.5	18.2
75	−19.8	−0.7	12.1	18.0	16.3	20.0	−96.8	−19.4	−15.3	3.0
76	−16.8	4.3	14.2	21.0	18.7	22.8	−94.7	−15.1	−13.3	6.9
77	−18.1	2.9	11.8	18.5	16.2	20.2	−93.7	−15.4	−14.9	4.8
78	−18.3	1.0	12.9	19.0	17.3	20.9	−95.4	−17.8	−14.1	4.4
79	−16.3	5.7	14.6	22.1	19.3	23.6	−94.5	−13.6	−13.0	8.2
80	−16.5	4.6	13.1	19.8	17.4	21.4	−92.1	−13.7	−13.4	6.3
81	−18.0	2.0	13.0	19.6	17.4	21.4	−95.2	−16.8	−14.0	5.2
82	−15.4	6.7	15.5	22.9	20.1	24.4	−93.6	−12.6	−12.1	9.1
83	−16.5	4.8	13.5	20.7	18.0	22.0	−92.8	−13.9	−13.1	7.0
84	−17.1	3.0	13.9	20.5	18.3	22.3	−94.2	−15.8	−13.1	6.3
85	−12.6	11.6	−2.3	15.7	24.2	24.7	−16.9	13.3	17.3	21.1
86	−7.8	15.6	2.5	19.8	28.4	29.0	−11.5	17.2	21.6	25.4
87	−1.3	17.1	5.9	19.8	30.7	31.3	−4.7	17.1	24.4	27.7
88	−7.3	14.9	2.7	19.0	28.0	28.5	−10.4	16.3	21.4	24.9
89	−11.8	12.4	−2.0	16.0	24.3	24.9	−16.4	13.7	17.4	21.4
90	−7.7	16.7	2.6	20.3	28.2	28.8	−10.9	18.0	21.4	25.4
91	−11.9	12.5	−2.1	16.1	24.2	25.0	−16.5	13.8	17.3	21.5
92	−7.5	16.8	2.7	20.4	28.3	28.9	−10.7	18.1	21.5	25.5
93	−6.8	16.7	3.1	20.5	29.1	29.7	−10.9	17.9	22.3	26.2

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Table 13 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
94	−6.7	16.7	3.3	20.5	29.2	29.7	−10.8	17.9	22.4	26.2
95	−8.5	16.7	0.4	19.6	27.0	27.6	−13.5	17.4	19.9	24.2
96	−6.5	17.9	3.6	21.4	29.2	29.9	−9.9	19.1	22.4	26.6
97	−8.4	17.1	0.4	20.0	27.3	28.0	−13.6	18.0	20.1	24.6
98	1.1	19.7	7.4	21.4	31.5	32.3	−2.9	19.2	25.4	28.9
99	−5.2	17.9	3.8	21.2	28.7	29.5	−9.5	18.5	22.1	26.1
100	−5.6	18.2	4.1	21.8	30.3	31.0	−9.9	19.2	23.4	27.4
101	−1.3	18.9	6.5	22.1	29.5	30.1	−5.3	18.8	23.1	27.0
102	−6.6	17.7	3.6	21.3	29.3	29.9	−10.1	18.8	22.5	26.6
103	−7.4	18.8	1.6	21.4	28.3	29.1	−12.3	19.4	21.2	25.8
104	−6.4	17.8	3.8	21.3	29.5	30.0	−9.9	18.9	22.7	26.6
105	−4.3	17.8	5.2	21.5	30.2	30.8	−7.8	18.8	23.7	27.4
106	−5.3	18.3	4.5	21.9	30.6	31.0	−9.6	19.3	23.7	27.6
107	−14.3	17.2	2.0	24.7	30.0	33.6	−45.4	16.0	18.3	28.1
108	−18.3	5.9	−2.9	16.0	22.2	25.2	−47.0	5.7	11.7	19.5
109	−13.2	20.1	3.0	27.2	31.8	35.9	−44.9	18.3	20.0	30.4
110	−13.4	18.7	1.7	24.7	28.7	32.6	−42.5	16.9	17.6	27.6
111	−16.0	10.0	−1.2	19.3	24.8	28.2	−46.0	9.2	14.1	22.8
112	−11.9	22.3	4.3	29.2	33.4	37.5	−44.1	20.1	21.4	32.1
113	−12.7	19.3	2.3	25.2	29.2	33.0	−42.1	17.3	18.2	28.1
114	−15.4	11.9	−0.6	20.8	26.0	29.7	−45.8	10.8	15.0	24.3
115	−11.5	22.7	4.7	29.5	33.8	37.8	−43.8	20.4	21.8	32.5
116	−12.5	19.5	2.6	25.5	29.6	33.4	−42.0	17.4	18.6	28.5
117	−15.1	12.3	−0.4	21.1	26.2	29.9	−45.7	11.1	15.3	24.7
118	−7.9	15.9	0.6	21.2	30.5	34.7	−27.2	12.9	24.9	30.2
119	−7.2	17.2	1.2	19.6	26.1	30.8	−24.8	12.2	21.9	26.6
120	−10.2	11.1	−2.5	17.3	27.4	31.6	−29.1	8.8	22.0	27.1
121	−8.7	17.5	1.3	20.2	27.0	31.5	−26.3	13.3	22.4	27.3
122	−4.8	20.3	3.2	25.0	33.1	38.0	−25.5	17.1	27.6	33.5
123	−7.9	19.0	0.8	21.5	27.6	32.5	−25.7	13.6	23.6	28.5
124	−8.3	16.5	0.3	21.3	30.8	35.2	−29.9	13.8	25.3	30.9
125	−7.6	21.5	2.2	23.4	29.2	33.9	−25.1	16.6	24.7	30.0

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Table 13 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
126	−8.1	19.0	1.3	21.1	27.3	32.1	−25.6	14.3	23.0	28.0
127	−6.0	21.6	3.8	26.1	34.6	39.4	−26.7	18.4	29.0	34.9
128	−39.0	8.7	−13.9	16.1	18.2	23.0	−46.7	8.1	11.3	19.5
129	−39.2	4.3	−15.3	12.2	14.4	19.0	−45.6	4.5	8.0	15.5
130	−37.9	9.9	−13.8	16.6	18.3	23.7	−46.1	8.8	11.6	20.2
131	−37.6	8.4	−14.9	15.1	16.4	21.5	−45.3	7.7	10.2	18.5
132	−38.1	5.8	−14.7	13.2	15.3	20.2	−45.0	5.6	9.1	16.8
133	−37.9	11.6	−13.6	18.2	19.6	25.3	−46.7	10.4	12.7	21.8
134	−37.5	8.4	−15.0	15.0	16.2	21.4	−45.4	7.6	10.2	18.5
135	−37.7	6.6	−14.8	13.8	15.5	20.8	−45.2	6.2	9.2	17.5
136	−37.4	12.1	−13.1	18.6	20.0	25.7	−46.3	10.8	13.2	22.3
137	−37.0	9.0	−14.6	15.5	16.7	22.0	−45.1	8.0	10.7	19.2
138	−37.3	7.4	−14.5	14.5	16.0	21.5	−45.0	6.8	9.8	18.2
139	−5.7	22.3	9.2	28.3	31.9	35.4	−34.4	22.6	23.1	31.9
140	−3.4	27.3	11.3	32.8	35.4	39.3	−32.9	26.7	26.2	36.0
141	−4.3	24.1	9.3	28.8	31.1	34.5	−31.8	23.5	22.9	31.6
142	−45.3	−8.9	−30.8	1.4	18.7	20.5	−48.0	−5.6	4.6	13.0
143	−43.1	−10.1	−29.7	0.2	17.6	19.4	−44.4	−5.5	3.6	11.6
144	−42.6	−11.0	−29.7	0.0	17.7	19.6	−43.9	−5.9	3.9	11.8
145	−46.9	−12.2	−32.0	−1.5	16.5	18.2	−49.2	−8.8	3.4	11.2
146	−44.8	−13.4	−31.2	−2.8	15.3	16.9	−46.1	−8.9	2.1	9.5
147	−45.5	−14.2	−31.1	−2.5	16.1	17.8	−46.1	−8.7	2.9	10.3
148	−16.7	−5.4	12.0	16.3	14.0	16.8	−76.2	−26.2	−14.9	−1.6
149	−20.6	1.5	9.0	15.9	10.1	14.2	−99.8	−27.0	−22.1	−1.5
150	−39.2	−7.4	−27.8	1.4	18.1	20.8	−44.8	−3.6	4.9	12.6
151	−16.2	23.1	−14.1	24.6	31.2	36.2	−29.5	20.5	18.9	30.1
152	−12.9	6.8	−2.0	15.3	17.3	20.6	−34.6	4.4	9.9	15.9
153	−0.3	26.0	5.4	26.1	25.1	29.5	−27.0	15.3	17.8	25.4
154	−17.0	2.8	0.7	16.4	21.8	24.6	−36.5	3.6	11.3	18.2
155	−11.8	14.4	0.5	21.4	25.0	28.6	−32.4	11.6	17.5	24.0
156	−0.4	26.4	11.9	30.6	30.6	34.5	−27.5	22.0	21.4	30.1
157	−8.9	20.0	1.4	23.5	28.1	32.2	−30.6	14.9	20.2	27.1

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Table 13 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
158	−16.5	−5.2	11.9	16.2	14.6	17.4	−76.1	−25.9	−14.4	−1.0
159	−16.7	−5.3	11.6	16.0	14.3	17.1	−76.6	−26.4	−14.8	−1.4
160	−38.7	−7.0	−27.7	1.5	18.7	21.3	−44.6	−3.6	5.3	13.0
161	−12.7	27.5	−11.2	28.5	35.0	39.7	−24.6	26.1	22.2	33.8
162	−16.5	0.8	−4.4	12.2	16.2	19.0	−33.7	−2.0	8.1	13.2
163	0.6	28.7	8.5	30.6	30.3	35.3	−26.5	21.3	22.6	30.6
164	−20.2	−0.1	−3.8	13.0	19.1	21.3	−36.0	0.8	8.9	15.1
165	−16.5	1.3	−2.7	13.5	18.3	21.0	−33.9	−0.2	9.9	15.0
166	−5.2	26.6	10.4	31.4	33.9	38.1	−33.9	22.7	23.0	33.0
167	−16.6	11.9	−2.1	20.0	25.2	28.9	−37.5	7.5	16.9	23.5
168	−16.3	−5.0	12.1	16.5	15.0	17.9	−76.1	−25.6	−13.9	−0.5
169	−16.4	−4.8	12.1	16.6	15.0	17.8	−76.9	−25.6	−14.2	−0.6
170	−39.7	−8.5	−28.3	0.3	16.7	19.5	−44.8	−4.7	3.6	11.3
171	−39.6	0.8	−31.4	7.0	20.7	24.5	−50.3	1.3	6.1	16.9
172	−11.9	7.7	1.8	19.8	21.2	24.9	−35.4	4.7	12.8	19.0
173	−6.7	24.6	3.7	28.7	28.9	33.7	−35.9	19.4	20.5	29.4
174	−17.3	0.0	−3.6	12.6	17.8	20.5	−34.4	−1.0	9.8	14.7
175	−12.9	21.8	5.8	29.4	32.7	37.1	−41.8	19.8	21.1	31.8
176	−11.3	19.6	4.8	26.7	30.9	35.6	−36.9	19.0	21.8	31.2
177	−15.8	−4.5	12.5	16.9	15.4	18.3	−75.3	−25.2	−13.4	−0.1
178	−15.2	12.6	14.5	22.9	16.9	21.8	−99.4	−10.3	−15.9	8.7
179	−39.3	−8.2	−28.1	0.6	17.0	19.8	−44.5	−4.5	4.0	11.7
180	−39.4	−7.7	−28.5	0.8	18.1	20.8	−45.4	−4.4	4.7	12.5
181	−11.4	15.7	1.9	25.0	25.8	30.4	−38.8	11.7	17.3	25.2
182	−10.1	18.2	2.9	26.7	27.2	32.1	−38.1	14.1	18.8	27.1
183	−18.9	1.1	−2.6	14.1	20.2	22.5	−34.8	1.7	10.1	16.3
184	−16.7	0.4	−3.1	13.0	18.2	20.9	−33.8	−0.6	10.1	15.1
185	−12.4	18.1	5.5	27.7	31.2	35.3	−40.4	16.8	20.0	29.9
186	−14.4	11.1	1.4	21.5	26.4	30.5	−37.7	11.6	17.4	25.8
187	−18.3	2.9	14.3	21.2	17.7	21.7	−94.5	−20.7	−15.7	4.5
188	−40.4	3.2	−30.7	8.9	23.9	27.7	−51.9	1.4	8.9	19.6
189	−13.7	15.9	1.2	26.6	27.3	31.9	−42.9	10.4	17.7	26.0

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Table 13 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
190	−17.1	15.1	2.4	26.0	30.8	34.5	−47.1	12.2	18.2	28.3
191	−18.4	8.7	−1.3	20.4	26.2	30.0	−43.8	6.9	15.8	24.3
192	−16.6	7.8	17.0	24.8	20.7	25.2	−96.4	−14.4	−13.5	8.9
193	−41.8	3.4	−32.6	9.1	23.8	27.8	−54.1	2.2	8.5	19.9
194	−13.8	17.8	1.5	28.6	28.5	33.6	−44.3	12.0	19.0	27.8
195	−18.0	16.3	3.2	27.7	32.0	36.1	−49.3	13.5	19.3	29.9
196	−19.4	9.5	−0.9	21.9	27.2	31.3	−46.2	8.4	16.9	25.9
197	−13.2	11.7	18.7	26.2	23.3	27.8	−95.2	−4.7	−9.8	13.0
198	−33.6	17.2	−28.0	17.3	28.7	32.8	−46.1	16.0	14.2	26.4
199	−6.6	28.5	3.5	32.6	33.4	38.6	−37.8	23.7	24.3	33.8
200	−6.6	32.9	9.8	37.1	39.7	44.2	−39.9	30.4	27.4	39.0
201	−14.3	25.8	0.5	30.8	35.3	40.0	−38.0	22.8	26.1	35.0
202	−17.6	0.8	12.5	19.1	15.4	19.2	−85.5	−23.7	−17.0	1.5
203	−44.7	−4.3	−34.5	2.9	19.4	22.8	−53.5	−3.1	4.3	14.3
204	−18.1	5.7	−4.5	16.9	19.9	23.6	−40.8	0.8	10.5	17.3
205	−19.7	6.1	−1.0	18.9	24.6	27.7	−44.4	4.6	12.7	21.1
206	−22.7	−1.5	−5.6	12.3	19.4	22.4	−44.4	−1.7	9.6	16.6
207	−16.6	5.5	14.5	21.2	17.9	21.9	−93.0	−10.8	−13.5	6.6
208	−32.7	12.8	−26.8	13.2	24.2	27.9	−42.1	12.8	10.8	21.5
209	−10.4	18.7	1.1	25.1	26.3	30.5	−38.7	15.6	18.1	25.8
210	−12.4	19.5	3.5	26.1	29.9	33.5	−41.4	18.6	19.1	28.5
211	−8.0	18.7	3.8	23.6	27.7	31.4	−31.0	18.7	19.2	27.4
212	−19.3	−3.3	10.2	16.0	13.0	16.2	−85.8	−27.4	−18.7	−2.4
213	−44.2	−8.4	−34.1	0.0	17.9	21.0	−52.4	−6.4	3.1	12.0
214	−17.0	8.3	−0.6	21.0	23.1	27.2	−43.3	5.0	13.7	20.9
215	−22.1	0.7	−2.3	15.4	22.5	25.5	−46.0	0.3	11.1	18.5
216	−23.4	0.4	−5.9	14.5	20.7	23.8	−44.0	−2.1	11.3	17.1
217	−18.7	0.1	12.9	19.3	15.6	19.2	−90.9	−22.6	−17.0	1.1
218	−46.3	−5.7	−36.1	2.2	19.1	22.7	−55.7	−4.0	3.7	13.9
219	−14.8	13.4	1.1	25.2	26.1	30.6	−42.9	9.7	16.4	24.3
220	−19.3	8.7	−0.8	21.7	26.7	29.8	−43.5	6.4	14.7	23.0
221	−25.3	5.0	−6.1	18.5	24.9	28.7	−45.5	3.1	15.3	22.2

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Table 13 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
222	−12.0	15.3	19.0	26.7	23.7	28.0	−91.7	2.9	−9.4	14.0
223	−44.7	−4.3	−35.1	3.1	20.1	23.8	−54.7	−3.3	4.8	15.0
224	−10.4	22.5	0.3	26.8	29.2	33.7	−40.4	19.6	20.1	29.1
225	−19.3	5.4	−1.8	18.0	24.3	27.2	−41.4	3.0	12.6	20.3
226	−19.6	6.1	−2.2	18.9	25.4	29.1	−44.9	5.7	14.8	23.3
227	−20.7	−4.3	10.2	15.6	12.2	15.3	−91.1	−26.6	−19.5	−3.4
228	−44.2	−13.6	−34.7	−5.4	12.1	14.7	−50.3	−10.7	−1.2	6.4
229	−21.8	1.5	−7.8	12.6	15.9	19.0	−44.4	−1.9	6.2	12.9
230	−23.3	−2.4	−8.9	8.4	14.3	16.3	−37.9	−2.9	4.2	10.7
231	−22.4	−6.4	−3.5	9.4	15.9	18.7	−39.7	−4.4	7.2	12.8
232	−19.3	−2.3	11.6	17.1	13.9	17.1	−90.9	−24.2	−17.8	−1.2
233	−43.4	−4.5	−33.0	3.1	19.8	23.2	−52.0	−2.4	5.3	14.8
234	−13.8	13.0	1.7	24.9	25.6	29.7	−41.9	10.0	16.1	23.6
235	−22.8	4.2	−5.2	16.6	23.8	26.5	−46.0	2.9	12.1	20.0
236	−21.9	−0.4	−6.3	12.8	18.0	21.1	−40.0	−3.2	9.4	14.6
MAXD	−52.2	54.6	−36.1	58.5	59.9	68.9	−99.8	51.4	56.0	64.9
MD	−16.4	14.7	0.3	22.5	26.6	30.4	−40.9	10.5	14.2	23.8
MAD	18.8	16.5	12.2	22.6	26.6	30.4	41.8	16.6	19.0	23.9

Table 14: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the B3LYP functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−20.8	24.5	−7.2	25.2	23.6	29.1	−16.7	24.2	21.4	28.0
2	−25.8	25.1	−10.0	26.0	24.2	30.3	−20.2	25.8	21.9	29.4
3	−22.8	22.7	−9.1	23.3	22.6	28.3	−18.4	22.9	20.3	27.1
4	−26.4	26.1	−10.4	27.0	25.2	31.5	−21.0	26.8	23.0	30.5
5	−24.4	24.8	−9.9	25.3	24.3	30.3	−19.9	24.8	22.1	29.2
6	−26.5	26.6	−10.6	27.4	25.6	32.0	−21.3	27.2	23.4	31.0
7	−24.2	25.0	−9.7	25.5	24.6	30.5	−19.9	24.9	22.3	29.4

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Table 14 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
8	−3.6	16.6	20.3	26.0	18.3	22.4	−75.9	−3.1	−6.7	11.8
9	−3.1	18.4	21.3	27.4	19.7	24.1	−77.7	0.7	−6.1	13.6
10	−14.3	0.2	13.9	18.4	12.9	16.2	−78.2	−17.0	−11.9	3.1
11	−12.0	3.2	15.1	19.7	14.5	17.9	−77.8	−13.2	−10.0	5.5
12	−3.0	17.3	20.7	26.5	19.0	23.3	−75.9	−2.4	−6.2	12.4
13	−1.4	20.3	22.9	29.2	21.5	26.0	−76.3	2.4	−3.6	16.0
14	−13.8	0.7	14.2	18.8	13.1	16.6	−78.0	−16.7	−11.2	3.5
15	−9.8	7.7	17.6	22.7	17.2	21.0	−78.5	−7.0	−7.7	9.1
16	−0.4	21.8	23.5	29.8	22.2	26.7	−75.6	2.2	−3.1	16.7
17	−1.0	20.8	23.4	29.8	22.0	26.5	−76.1	2.9	−3.3	16.8
18	−13.2	1.9	14.9	19.9	14.0	17.5	−77.7	−15.4	−10.7	5.0
19	−9.1	9.2	18.3	23.8	18.0	21.8	−78.5	−5.2	−7.2	10.2
20	0.0	22.3	23.9	30.2	22.7	27.2	−75.6	2.6	−2.7	17.3
21	14.1	35.3	19.8	35.7	37.9	39.9	10.3	34.9	34.5	37.7
22	−4.2	11.1	3.9	17.0	22.7	24.0	−4.9	15.0	19.5	22.1
23	14.6	36.5	20.6	37.4	40.1	42.0	11.3	36.0	35.7	39.7
24	12.5	34.4	18.6	35.3	37.6	39.2	8.9	33.9	33.3	37.2
25	12.6	35.5	19.0	36.3	38.5	40.4	8.7	34.9	34.3	38.6
26	12.8	33.8	18.6	34.5	37.1	38.9	9.4	33.2	33.1	37.3
27	13.8	35.0	19.4	35.3	37.9	39.8	9.9	34.3	33.8	37.8
28	15.8	37.1	21.2	37.2	39.3	41.3	12.1	36.3	35.4	39.6
29	15.1	37.2	21.1	38.0	40.7	42.6	11.9	36.6	36.5	40.4
30	15.0	39.5	21.7	39.7	41.6	43.6	11.7	38.6	37.6	41.7
31	3.7	22.8	11.5	26.8	32.0	33.5	2.2	25.6	27.9	31.3
32	14.2	39.1	20.9	39.6	41.5	43.5	10.5	38.5	37.3	41.7
33	17.1	38.4	22.4	38.4	40.6	42.8	13.2	37.1	36.8	41.2
34	16.5	37.8	21.8	37.8	39.9	41.9	12.6	36.7	36.1	39.8
35	16.5	38.8	22.4	39.6	42.3	44.2	13.0	38.1	38.0	42.1
36	16.6	42.1	23.4	42.5	44.3	46.3	12.9	41.4	40.2	44.5
37	18.6	39.9	23.8	39.9	42.1	44.3	14.8	38.6	38.2	42.0
38	3.8	34.8	12.3	33.0	33.4	38.4	−22.6	29.5	27.3	38.1
39	4.2	36.6	15.0	36.3	35.4	40.8	−25.5	32.6	28.2	37.4

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Table 14 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
40	3.9	35.2	12.5	33.6	34.2	39.5	−23.1	29.7	27.4	38.9
41	4.6	38.9	15.7	38.6	37.6	43.1	−26.1	34.9	30.5	39.9
42	4.5	35.9	13.0	34.2	34.9	40.2	−23.0	30.0	28.4	39.6
43	5.4	40.3	16.4	39.9	38.7	44.4	−25.7	36.0	31.4	41.1
44	4.3	35.8	12.8	34.0	34.8	40.2	−23.2	29.8	28.4	37.1
45	13.0	42.2	20.4	44.0	44.9	52.7	−5.0	37.5	44.2	50.0
46	−9.2	5.2	−4.1	11.5	19.7	23.7	−22.9	3.6	17.3	21.1
47	4.0	27.8	11.1	28.4	30.8	36.8	−9.4	23.2	29.3	33.9
48	13.3	46.9	22.0	49.6	49.3	58.2	−5.3	42.6	49.0	55.9
49	−8.1	14.8	0.2	20.9	27.5	32.8	−21.1	13.4	25.5	30.0
50	2.7	29.1	11.4	30.0	32.5	39.1	−12.1	25.1	30.8	35.8
51	11.8	40.7	19.8	42.3	44.2	51.7	−5.1	36.2	43.1	48.9
52	14.2	49.7	23.5	52.3	51.6	61.0	−4.2	45.5	51.8	58.5
53	−6.8	18.4	2.1	24.0	30.5	36.3	−20.5	17.1	28.6	33.4
54	2.6	30.5	12.1	31.3	33.8	40.6	−12.2	26.4	32.3	37.2
55	13.0	42.3	21.1	43.5	44.6	52.1	−3.0	37.3	44.1	49.7
56	−12.5	27.9	4.1	29.3	24.3	30.5	−19.7	23.4	22.2	28.8
57	−16.8	30.2	2.2	32.0	26.0	33.0	−23.6	26.2	24.4	31.6
58	−12.7	27.7	3.7	28.9	24.1	30.6	−19.9	23.2	22.4	28.9
59	−13.7	31.1	2.7	31.2	25.1	32.2	−23.2	25.8	23.6	31.0
60	−12.7	27.7	3.5	28.9	24.2	30.7	−20.1	23.0	22.7	29.1
61	−16.8	33.1	2.7	34.7	28.3	35.9	−24.1	29.1	26.8	34.6
62	−12.7	27.7	3.6	28.9	24.2	30.8	−20.2	23.0	22.7	29.3
63	12.8	44.8	22.1	43.6	41.0	46.4	−15.8	42.3	36.0	44.8
64	−41.5	4.6	−23.4	10.4	15.6	19.9	−32.3	10.9	12.4	18.5
65	−40.6	−0.6	−24.0	6.0	11.9	15.9	−30.9	6.6	9.4	14.9
66	−40.6	6.1	−23.1	11.5	16.6	21.1	−32.1	11.9	13.1	19.7
67	−38.8	4.8	−23.0	10.0	14.0	18.5	−31.0	10.5	11.6	17.8
68	−40.1	0.7	−23.6	7.1	12.9	17.2	−30.8	7.7	10.6	16.2
69	−40.7	6.7	−23.7	11.9	16.6	21.3	−32.8	12.2	14.2	20.4
70	−39.5	4.6	−23.5	9.8	13.9	18.5	−31.8	10.3	12.2	17.8
71	−39.9	1.0	−23.9	7.2	12.8	17.3	−31.2	7.7	10.9	16.4

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Table 14 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
72	−40.2	7.3	−23.2	12.4	17.1	21.9	−32.4	12.7	13.9	20.6
73	−39.0	5.0	−23.2	10.2	14.3	19.0	−31.5	10.5	12.7	18.1
74	−39.9	1.2	−23.9	7.4	13.0	17.6	−31.3	7.8	10.6	16.3
75	−13.9	1.1	14.7	19.2	14.5	17.8	−83.3	−16.7	−10.2	4.6
76	−11.2	5.4	16.5	21.6	16.7	20.3	−81.2	−13.1	−8.1	7.8
77	−12.3	4.2	14.2	19.2	14.6	18.2	−80.2	−13.1	−9.3	6.0
78	−12.8	2.4	15.3	19.8	15.3	18.6	−82.2	−15.6	−9.1	5.5
79	−10.8	6.5	16.8	22.3	17.2	21.0	−81.1	−11.9	−7.7	8.6
80	−10.8	5.7	15.4	20.4	15.8	19.4	−78.6	−11.6	−8.2	7.3
81	−12.6	3.1	15.3	20.3	15.5	19.0	−82.0	−14.9	−8.7	6.3
82	−10.0	7.4	17.5	23.1	17.9	21.8	−80.3	−11.0	−6.9	9.6
83	−10.8	5.8	15.8	21.1	16.3	19.9	−79.4	−12.0	−7.6	8.3
84	−11.7	4.0	16.1	21.1	16.3	19.9	−81.2	−14.0	−7.8	7.3
85	−6.9	12.8	1.4	16.1	22.2	22.9	−9.5	14.9	17.6	20.4
86	−2.6	16.4	5.5	19.7	25.6	26.4	−4.6	18.4	21.2	23.9
87	0.9	15.5	6.3	17.8	27.0	27.7	−1.6	15.9	22.5	25.2
88	−2.6	15.4	5.4	18.7	25.0	25.7	−4.2	17.4	20.4	23.3
89	−6.2	13.5	1.7	16.4	22.4	23.1	−9.1	15.2	17.7	20.8
90	−2.4	17.4	5.7	20.3	25.5	26.4	−4.0	19.3	21.0	24.0
91	−6.3	13.5	1.6	16.5	22.3	23.2	−9.1	15.3	17.7	20.8
92	−2.3	17.5	5.8	20.4	25.6	26.5	−3.8	19.4	21.2	24.2
93	−1.8	17.2	6.1	20.3	26.2	27.0	−4.1	19.0	21.6	24.5
94	−1.7	17.2	6.2	20.3	26.3	27.0	−4.0	19.0	21.7	24.4
95	−2.8	17.6	4.2	19.9	25.0	25.8	−6.0	18.9	20.4	23.2
96	−1.4	18.5	6.7	21.3	26.5	27.4	−3.0	20.4	21.9	25.1
97	−2.8	17.9	4.2	20.1	25.2	26.0	−6.1	19.3	20.6	23.5
98	2.9	17.9	7.7	19.3	27.7	28.7	0.0	17.9	23.9	26.3
99	−0.2	18.5	6.9	21.1	26.3	27.2	−2.9	19.7	22.1	24.8
100	−0.7	18.5	7.0	21.5	27.4	28.2	−3.3	20.2	23.1	26.2
101	3.0	19.5	9.1	22.0	27.0	27.8	0.5	20.1	22.9	25.5
102	−1.6	18.3	6.6	21.2	26.6	27.4	−3.3	20.0	22.3	25.3
103	−1.8	19.4	5.3	21.4	26.1	27.1	−4.9	20.6	21.7	24.9

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Table 14 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
104	−1.4	18.3	6.8	21.2	26.8	27.5	−3.1	20.1	22.3	25.4
105	−0.2	17.8	7.6	21.0	27.1	27.9	−2.1	19.5	22.7	25.7
106	−0.5	18.6	7.3	21.5	27.6	28.3	−3.0	20.2	23.3	25.7
107	−12.1	13.9	0.4	19.8	23.6	27.4	−38.7	13.0	15.6	23.3
108	−16.0	4.0	−4.0	12.4	16.9	20.1	−40.8	3.7	10.0	16.0
109	−11.1	16.4	1.3	22.0	25.2	29.3	−38.2	15.0	17.4	25.6
110	−11.0	15.5	0.5	20.1	22.7	26.6	−35.9	14.1	15.4	23.1
111	−13.9	7.7	−2.3	15.4	19.2	22.8	−39.8	6.9	12.2	18.9
112	−9.8	18.5	2.6	23.9	26.7	30.8	−37.5	16.7	19.0	27.0
113	−10.4	16.0	1.0	20.6	23.2	27.1	−35.5	14.5	16.0	23.5
114	−13.2	9.4	−1.6	16.7	20.4	24.2	−39.5	8.4	13.4	20.3
115	−9.5	18.8	2.9	24.2	27.0	31.2	−37.2	17.0	19.4	27.5
116	−10.2	16.2	1.2	20.8	23.5	27.4	−35.6	14.5	16.1	24.1
117	−13.0	9.7	−1.5	17.0	20.5	24.5	−39.5	8.6	13.7	20.7
118	−3.3	16.0	2.5	20.4	27.3	31.7	−18.3	14.1	24.5	29.1
119	−2.2	17.0	3.1	18.2	22.6	27.5	−16.6	12.8	20.7	24.8
120	−5.7	11.7	−0.5	16.8	24.6	29.0	−20.2	10.3	21.9	26.4
121	−3.6	16.8	3.0	18.4	23.1	27.8	−17.9	13.5	20.7	25.0
122	−0.2	20.0	5.2	23.8	29.7	34.8	−16.7	17.9	27.3	31.8
123	−2.1	19.0	3.5	20.4	24.3	29.5	−16.5	14.6	22.4	26.2
124	−3.3	16.6	2.2	20.5	27.7	32.3	−20.4	14.9	24.8	29.8
125	−1.7	21.2	4.7	21.9	25.6	30.6	−15.6	17.1	23.3	28.1
126	−2.8	18.4	3.3	19.4	23.6	28.6	−16.8	14.5	21.5	25.5
127	−1.0	21.1	5.6	24.8	31.0	36.1	−17.4	19.0	28.6	32.6
128	−29.4	9.3	−8.9	15.1	15.1	19.9	−33.5	9.3	11.9	18.1
129	−30.1	5.2	−10.3	11.6	11.7	16.2	−33.2	5.8	9.0	14.5
130	−28.3	10.4	−8.6	15.7	15.5	20.7	−32.9	10.1	12.9	19.3
131	−28.0	9.3	−9.6	14.4	13.9	18.9	−32.3	9.2	11.4	17.8
132	−29.1	6.5	−9.7	12.6	12.6	17.5	−32.6	7.0	10.3	16.0
133	−28.3	11.9	−8.3	17.1	16.5	22.0	−33.3	11.4	14.0	20.2
134	−28.0	9.2	−9.6	14.3	13.7	18.8	−32.4	9.1	11.9	17.9
135	−28.7	7.2	−9.7	13.1	12.9	18.1	−32.7	7.5	11.0	16.7

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Table 14 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
136	−27.8	12.3	−7.9	17.5	16.9	22.5	−33.0	11.8	14.2	20.8
137	−27.5	9.8	−9.2	14.8	14.2	19.4	−32.1	9.5	12.4	18.6
138	−28.3	7.9	−9.4	13.7	13.3	18.6	−32.5	8.0	11.2	17.5
139	−6.4	16.7	5.0	21.8	24.6	28.2	−31.1	17.1	18.9	25.8
140	−4.2	21.3	7.2	26.0	27.8	31.9	−29.7	21.0	22.3	29.4
141	−4.8	18.7	5.6	22.6	24.2	27.8	−28.5	18.3	19.2	25.7
142	−38.8	−9.2	−26.6	−0.2	13.9	15.6	−40.7	−6.0	3.6	10.2
143	−37.1	−10.4	−25.8	−1.2	12.6	14.5	−37.6	−5.8	2.5	8.6
144	−36.2	−10.5	−25.6	−1.1	12.8	14.8	−36.9	−5.7	3.1	8.7
145	−38.4	−10.5	−25.8	−1.0	13.1	14.9	−39.7	−7.0	3.8	9.8
146	−36.9	−11.6	−25.2	−2.2	11.9	13.6	−37.0	−6.9	2.5	8.2
147	−37.2	−12.0	−25.1	−1.7	12.5	14.3	−36.9	−6.5	3.3	9.0
148	−11.7	−2.6	13.3	16.7	11.5	14.0	−65.6	−22.9	−11.1	−0.5
149	−13.3	4.2	11.7	17.0	9.4	13.1	−85.5	−23.5	−16.0	0.4
150	−31.7	−6.2	−22.5	1.2	13.9	16.5	−35.6	−2.7	5.7	10.9
151	−7.8	24.7	−7.0	25.0	28.0	32.8	−18.5	22.5	20.4	28.8
152	−8.2	7.5	0.3	15.0	14.1	17.5	−26.2	5.8	10.4	14.5
153	5.4	26.5	8.5	25.7	23.0	27.6	−17.1	17.3	19.2	24.7
154	−16.7	−0.2	−2.5	11.2	14.6	17.5	−33.6	0.5	7.8	12.9
155	−7.7	13.5	1.3	19.0	20.2	24.0	−24.5	11.5	16.1	21.0
156	0.5	22.8	9.5	25.6	24.2	28.2	−23.0	18.9	18.7	25.7
157	−4.4	18.9	2.6	21.0	23.4	27.7	−22.4	14.7	19.3	24.5
158	−11.7	−2.6	13.1	16.5	11.9	14.5	−65.7	−22.9	−10.9	−0.1
159	−11.8	−2.6	13.0	16.4	11.8	14.4	−65.9	−23.0	−11.1	−0.5
160	−31.5	−6.1	−22.4	1.2	14.4	17.0	−35.6	−2.7	5.7	11.1
161	−5.4	27.8	−4.9	27.9	30.8	35.4	−14.4	27.1	22.9	31.9
162	−11.9	1.8	−2.4	11.9	12.8	15.8	−26.1	−0.3	8.1	12.3
163	4.8	27.3	10.2	28.5	26.0	31.1	−18.1	21.2	22.4	28.1
164	−19.2	−2.6	−6.5	8.3	12.6	14.9	−32.8	−1.9	5.5	10.4
165	−12.4	1.9	−1.8	12.4	14.2	17.1	−26.6	1.2	9.1	12.3
166	−4.2	22.2	7.5	25.3	26.5	30.9	−29.1	18.7	19.7	27.5
167	−10.6	12.2	−0.1	18.7	21.0	25.0	−28.0	8.7	16.6	21.8

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Table 14 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
168	−11.7	−2.6	13.2	16.6	12.2	14.8	−65.8	−22.8	−10.6	0.1
169	−11.6	−2.2	13.3	16.9	12.3	15.0	−66.2	−22.5	−10.9	0.0
170	−32.1	−7.0	−22.7	0.4	12.9	15.6	−35.5	−3.4	4.3	9.7
171	−28.6	4.1	−22.4	8.8	18.5	22.1	−36.9	4.8	9.2	17.1
172	−7.1	8.8	4.2	19.6	17.4	21.3	−26.5	6.7	13.1	17.6
173	−1.2	23.7	6.2	26.9	24.8	29.7	−25.4	19.6	20.6	26.8
174	−13.5	0.4	−2.9	11.3	13.6	16.5	−27.4	0.2	8.6	11.7
175	−11.2	17.4	2.9	23.1	25.0	29.5	−36.2	15.5	17.4	25.9
176	−7.0	18.2	5.0	23.8	25.5	30.5	−28.1	18.3	20.3	27.6
177	−11.2	−2.1	13.5	17.0	12.6	15.3	−65.1	−22.4	−10.2	0.7
178	−7.8	14.2	17.0	23.3	15.9	20.3	−84.0	−7.8	−8.9	10.5
179	−31.9	−6.8	−22.5	0.7	13.1	15.9	−35.3	−3.2	4.8	9.9
180	−32.3	−6.9	−23.3	0.3	13.7	16.3	−36.5	−3.7	4.8	10.0
181	−5.6	16.0	4.8	24.2	21.8	26.7	−28.4	13.0	18.0	23.5
182	−4.4	18.2	5.6	25.7	23.1	28.1	−27.7	15.2	19.2	25.4
183	−18.2	−1.7	−5.5	9.1	13.5	15.9	−31.8	−1.3	6.7	11.6
184	−13.1	0.7	−2.5	11.6	13.9	16.8	−26.9	0.5	8.9	12.9
185	−11.3	14.0	2.5	21.6	23.6	27.8	−35.5	12.8	16.2	24.1
186	−10.3	10.6	1.9	19.4	21.4	25.7	−29.4	11.8	16.2	22.7
187	−12.2	4.6	16.3	21.4	15.5	19.2	−80.8	−18.0	−10.6	5.6
188	−30.6	4.5	−22.8	9.5	20.6	24.4	−39.6	3.5	11.0	18.8
189	−6.8	16.8	4.9	26.4	23.7	28.4	−31.1	12.7	18.7	24.5
190	−14.9	11.8	0.2	20.8	23.7	27.6	−40.8	9.4	15.2	23.0
191	−13.1	9.1	−0.1	19.1	21.8	25.8	−34.1	8.2	15.4	21.8
192	−10.8	8.5	18.4	24.3	18.0	22.1	−82.8	−12.8	−8.6	9.2
193	−31.9	4.3	−24.5	9.3	20.3	24.2	−41.6	3.7	10.3	19.0
194	−6.9	18.3	5.2	28.0	24.6	29.9	−32.2	14.0	19.8	26.1
195	−15.9	12.5	0.7	22.0	24.3	28.6	−42.9	10.1	15.8	24.1
196	−14.0	9.7	0.4	20.4	22.5	26.8	−36.1	9.5	16.2	23.1
197	−8.2	11.4	19.9	25.6	20.3	24.3	−82.0	−4.3	−5.4	12.5
198	−25.2	15.6	−21.0	15.8	24.3	28.3	−35.0	15.0	14.9	23.8
199	−1.0	26.7	6.1	30.2	28.7	33.9	−27.1	23.0	24.2	31.3

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Table 14 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
200	−5.5	27.1	6.6	30.1	31.4	36.0	−34.2	25.1	23.5	32.5
201	−8.5	23.7	2.2	27.7	29.8	34.7	−28.2	21.7	24.5	31.4
202	−11.9	2.7	14.7	19.6	13.5	17.0	−72.7	−20.6	−11.9	2.7
203	−35.2	−2.7	−26.6	3.8	16.2	19.5	−41.6	−1.0	6.3	13.6
204	−11.5	7.4	−0.5	17.6	17.1	21.0	−30.1	3.9	11.7	16.5
205	−17.9	3.5	−2.9	14.5	18.1	21.3	−38.9	2.5	9.6	16.1
206	−17.2	0.3	−3.6	12.3	16.0	19.2	−34.7	0.9	9.7	15.0
207	−11.5	5.9	16.2	21.2	15.6	19.2	−80.1	−9.6	−8.9	7.1
208	−25.0	11.5	−20.4	11.9	20.1	23.7	−31.8	12.3	11.6	19.9
209	−4.9	18.1	3.9	23.7	22.3	26.7	−28.1	16.1	18.5	24.1
210	−11.0	15.4	1.2	20.5	22.8	26.6	−35.7	14.9	15.7	23.1
211	−4.9	16.8	3.8	20.9	22.7	26.5	−23.4	18.0	17.8	24.5
212	−13.4	−0.7	12.7	17.0	11.4	14.4	−73.0	−23.6	−13.3	−0.4
213	−34.7	−5.7	−26.2	1.7	14.8	17.9	−40.4	−3.3	5.2	11.5
214	−9.9	10.3	3.4	21.7	19.9	24.2	−31.3	8.3	15.0	20.2
215	−20.0	−1.1	−4.1	11.4	16.0	19.2	−40.4	−1.2	8.4	14.3
216	−17.2	2.0	−3.2	14.2	16.6	20.0	−33.8	1.0	10.8	15.1
217	−13.0	1.8	14.9	19.8	13.5	16.9	−78.1	−19.9	−12.0	2.2
218	−36.8	−3.9	−28.2	3.2	15.6	19.2	−43.6	−1.6	5.9	13.0
219	−8.5	14.0	4.3	24.7	22.0	26.6	−31.5	11.7	17.0	22.5
220	−17.3	5.8	−2.7	16.9	19.7	23.0	−37.7	4.2	11.8	18.2
221	−18.7	5.7	−3.7	17.2	20.2	24.2	−34.9	4.8	14.5	18.7
222	−7.1	14.4	20.1	25.9	20.7	24.6	−78.4	2.8	−5.0	13.3
223	−35.6	−2.9	−27.5	3.7	16.3	19.9	−43.0	−1.3	6.8	14.0
224	−4.7	21.2	3.1	25.0	25.0	29.7	−29.4	19.3	20.5	27.9
225	−17.7	2.7	−3.8	13.5	17.6	20.7	−36.6	0.9	9.6	15.6
226	−15.3	5.7	−1.7	17.0	20.3	24.2	−35.9	6.3	13.9	20.1
227	−14.5	−1.5	12.8	16.9	10.6	13.5	−78.0	−23.0	−14.0	−1.2
228	−33.3	−8.7	−25.5	−1.8	10.9	13.5	−37.4	−5.6	2.7	7.8
229	−14.4	4.1	−3.1	14.1	13.8	17.0	−32.8	1.9	8.4	13.0
230	−20.5	−3.2	−9.1	5.9	10.0	12.1	−33.1	−3.7	3.0	8.5
231	−16.8	−3.5	−1.2	10.2	12.6	15.7	−30.5	−0.5	7.5	12.3

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Table 14 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
232	−13.4	0.0	13.8	18.0	12.1	15.0	−77.9	−21.0	−12.7	0.6
233	−34.2	−2.6	−25.6	4.0	16.2	19.6	−40.5	−0.2	7.1	14.3
234	−7.9	13.7	4.8	24.4	21.4	25.7	−30.8	11.9	17.1	22.8
235	−20.7	1.5	−7.1	12.0	17.0	19.9	−40.4	0.6	9.2	15.8
236	−16.1	1.4	−3.7	12.7	14.2	17.6	−30.8	−0.2	9.2	12.9
MAXD	−41.5	49.7	−28.2	52.3	51.6	61.0	−85.5	45.5	51.8	58.5
MD	−11.2	14.1	2.3	20.7	22.4	26.2	−32.1	10.4	14.1	21.5
MAD	14.3	15.4	11.3	20.7	22.4	26.2	33.6	15.6	17.2	21.5

Table 15: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the B3LYP-D3 functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−47.5	−2.2	−33.9	−1.6	−3.1	2.4	−43.4	−2.5	−5.3	1.3
2	−55.1	−4.2	−39.3	−3.3	−5.1	1.0	−49.5	−3.5	−7.4	0.1
3	−49.2	−3.7	−35.5	−3.0	−3.8	1.9	−44.8	−3.5	−6.1	0.7
4	−56.8	−4.2	−40.8	−3.4	−5.2	1.1	−51.4	−3.6	−7.4	0.1
5	−53.1	−3.9	−38.6	−3.4	−4.4	1.6	−48.6	−3.9	−6.6	0.5
6	−57.5	−4.4	−41.6	−3.6	−5.5	1.0	−52.3	−3.8	−7.6	0.0
7	−53.1	−4.0	−38.7	−3.5	−4.3	1.6	−48.8	−4.0	−6.7	0.5
8	−19.6	0.6	4.3	10.0	2.2	6.4	−91.9	−19.1	−22.8	−4.2
9	−20.1	1.4	4.3	10.4	2.8	7.1	−94.7	−16.3	−23.0	−3.4
10	−24.6	−10.1	3.6	8.1	2.5	5.9	−88.5	−27.3	−22.3	−7.3
11	−23.0	−7.9	4.0	8.7	3.5	6.9	−88.8	−24.2	−21.0	−5.5
12	−19.4	0.9	4.3	10.1	2.6	6.9	−92.3	−18.8	−22.6	−4.0
13	−18.8	2.9	5.6	11.8	4.1	8.6	−93.7	−15.0	−21.0	−1.4
14	−24.5	−10.0	3.5	8.1	2.4	5.9	−88.7	−27.3	−21.9	−7.2
15	−22.9	−5.4	4.5	9.7	4.2	7.9	−91.6	−20.1	−20.7	−4.0
16	−18.5	3.7	5.4	11.6	4.1	8.6	−93.7	−16.0	−21.2	−1.4

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Table 15 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
17	−18.8	3.1	5.6	12.0	4.3	8.8	−93.8	−14.9	−21.1	−1.0
18	−24.5	−9.4	3.6	8.6	2.7	6.2	−89.0	−26.7	−22.0	−6.3
19	−23.2	−5.0	4.2	9.7	3.9	7.7	−92.6	−19.3	−21.3	−3.9
20	−18.5	3.8	5.4	11.7	4.2	8.7	−94.1	−15.9	−21.2	−1.2
21	−16.5	4.7	−10.8	5.2	7.4	9.3	−20.2	4.3	3.9	7.1
22	−23.3	−8.1	−15.3	−2.1	3.6	4.8	−24.0	−4.2	0.4	3.0
23	−18.7	3.2	−12.6	4.2	6.9	8.7	−21.9	2.7	2.5	6.5
24	−19.1	2.8	−13.0	3.8	6.1	7.7	−22.7	2.4	1.7	5.6
25	−20.2	2.8	−13.8	3.5	5.8	7.7	−24.0	2.1	1.5	5.8
26	−17.8	3.2	−12.0	3.9	6.5	8.3	−21.2	2.6	2.5	6.7
27	−16.9	4.3	−11.3	4.5	7.1	9.0	−20.8	3.5	3.1	7.1
28	−15.5	5.7	−10.1	5.8	7.9	9.9	−19.2	5.0	4.1	8.3
29	−18.8	3.3	−12.8	4.1	6.8	8.7	−22.1	2.7	2.6	6.5
30	−20.6	3.8	−13.9	4.1	6.0	8.0	−23.9	2.9	1.9	6.1
31	−22.9	−3.9	−15.1	0.2	5.4	6.9	−24.4	−1.0	1.3	4.7
32	−21.2	3.7	−14.6	4.1	6.1	8.1	−24.9	3.1	1.9	6.3
33	−16.3	5.0	−11.1	5.0	7.2	9.4	−20.2	3.7	3.4	7.8
34	−15.1	6.1	−9.8	6.1	8.2	10.2	−19.0	5.1	4.5	8.2
35	−18.1	4.2	−12.1	5.1	7.8	9.7	−21.5	3.5	3.4	7.6
36	−20.1	5.4	−13.4	5.7	7.5	9.6	−23.9	4.7	3.4	7.8
37	−15.1	6.2	−9.8	6.2	8.4	10.6	−18.9	4.9	4.5	8.3
38	−32.8	−1.8	−24.4	−3.6	−3.2	1.8	−59.2	−7.1	−9.3	1.5
39	−35.2	−2.8	−24.5	−3.1	−4.1	1.3	−64.9	−6.8	−11.2	−2.0
40	−33.3	−2.0	−24.7	−3.6	−3.0	2.2	−60.3	−7.6	−9.8	1.7
41	−36.9	−2.5	−25.8	−2.8	−3.9	1.6	−67.6	−6.6	−10.9	−1.6
42	−33.1	−1.7	−24.6	−3.4	−2.7	2.6	−60.6	−7.6	−9.2	1.9
43	−37.3	−2.3	−26.2	−2.7	−4.0	1.7	−68.4	−6.6	−11.2	−1.6
44	−33.4	−1.9	−25.0	−3.7	−2.9	2.4	−60.9	−7.9	−9.3	−0.7
45	−39.5	−10.4	−32.1	−8.5	−7.6	0.1	−57.6	−15.1	−8.4	−2.5
46	−37.1	−22.7	−32.0	−16.5	−8.2	−4.3	−50.9	−24.3	−10.6	−6.8
47	−34.0	−10.3	−26.9	−9.7	−7.3	−1.2	−47.5	−14.8	−8.8	−4.2
48	−46.2	−12.7	−37.5	−10.0	−10.2	−1.3	−64.8	−17.0	−10.6	−3.7

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Table 15 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
49	−45.6	−22.6	−37.3	−16.5	−9.9	−4.6	−58.6	−24.1	−12.0	−7.4
50	−38.4	−12.0	−29.7	−11.1	−8.6	−2.0	−53.2	−16.0	−10.3	−5.3
51	−39.8	−10.9	−31.8	−9.3	−7.4	0.1	−56.7	−15.4	−8.5	−2.7
52	−48.5	−13.0	−39.2	−10.4	−11.1	−1.7	−66.9	−17.3	−10.9	−4.2
53	−48.1	−22.9	−39.2	−17.3	−10.8	−5.0	−61.8	−24.2	−12.7	−7.9
54	−40.3	−12.5	−30.9	−11.7	−9.2	−2.4	−55.2	−16.5	−10.6	−5.8
55	−38.9	−9.6	−30.8	−8.3	−7.3	0.3	−54.9	−14.6	−7.8	−2.1
56	−43.3	−3.0	−26.7	−1.5	−6.5	−0.4	−50.6	−7.4	−8.7	−2.1
57	−51.7	−4.7	−32.7	−2.9	−9.0	−1.9	−58.5	−8.7	−10.6	−3.3
58	−43.8	−3.4	−27.4	−2.1	−6.9	−0.5	−51.0	−7.9	−8.7	−2.1
59	−48.1	−3.3	−31.8	−3.2	−9.3	−2.2	−57.6	−8.7	−10.8	−3.4
60	−43.8	−3.5	−27.7	−2.3	−7.0	−0.4	−51.3	−8.2	−8.5	−2.1
61	−55.0	−5.1	−35.4	−3.4	−9.9	−2.2	−62.3	−9.1	−11.4	−3.6
62	−43.9	−3.6	−27.7	−2.4	−7.0	−0.5	−51.5	−8.3	−8.5	−2.0
63	−31.5	0.4	−22.3	−0.8	−3.4	2.1	−60.1	−2.1	−8.4	0.4
64	−65.6	−19.4	−47.5	−13.6	−8.5	−4.1	−56.4	−13.2	−11.7	−5.6
65	−61.7	−21.7	−45.0	−15.1	−9.2	−5.2	−52.0	−14.4	−11.6	−6.2
66	−65.7	−18.9	−48.1	−13.5	−8.5	−4.0	−57.1	−13.1	−12.0	−5.3
67	−60.6	−17.1	−44.8	−11.8	−7.8	−3.4	−52.8	−11.3	−10.2	−4.1
68	−61.7	−20.9	−45.3	−14.5	−8.8	−4.5	−52.5	−13.9	−11.1	−5.5
69	−66.6	−19.1	−49.5	−14.0	−9.3	−4.5	−58.7	−13.6	−11.7	−5.5
70	−61.8	−17.7	−45.8	−12.5	−8.4	−3.8	−54.1	−12.0	−10.1	−4.5
71	−62.2	−21.3	−46.1	−15.1	−9.4	−5.0	−53.4	−14.6	−11.3	−5.8
72	−66.2	−18.8	−49.3	−13.7	−8.9	−4.2	−58.5	−13.4	−12.1	−5.4
73	−61.6	−17.6	−45.8	−12.4	−8.3	−3.6	−54.1	−12.1	−10.0	−4.5
74	−62.4	−21.2	−46.3	−15.0	−9.5	−4.9	−53.8	−14.6	−11.9	−6.2
75	−25.8	−10.8	2.8	7.3	2.7	6.0	−95.2	−28.6	−22.0	−7.3
76	−25.1	−8.5	2.6	7.7	2.8	6.4	−95.1	−27.0	−22.0	−6.1
77	−25.2	−8.7	1.3	6.3	1.6	5.2	−93.1	−26.1	−22.3	−6.9
78	−25.2	−10.1	2.8	7.4	2.9	6.2	−94.6	−28.0	−21.5	−6.9
79	−25.2	−8.0	2.3	7.9	2.7	6.6	−95.5	−26.4	−22.2	−5.9
80	−24.1	−7.6	2.1	7.1	2.5	6.1	−91.9	−24.9	−21.5	−6.0

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Table 15 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
81	−25.5	−9.8	2.4	7.4	2.6	6.1	−94.9	−27.8	−21.6	−6.6
82	−24.5	−7.2	2.9	8.5	3.4	7.2	−94.8	−25.6	−21.5	−5.0
83	−24.4	−7.8	2.2	7.5	2.7	6.3	−93.0	−25.6	−21.3	−5.3
84	−24.7	−9.0	3.1	8.1	3.3	6.9	−94.2	−27.0	−20.8	−5.6
85	−29.8	−10.1	−21.4	−6.7	−0.6	0.1	−32.3	−7.9	−5.2	−2.4
86	−27.8	−8.9	−19.7	−5.6	0.4	1.1	−29.8	−6.8	−4.1	−1.4
87	−21.2	−6.6	−15.8	−4.3	4.9	5.6	−23.7	−6.2	0.4	3.1
88	−27.3	−9.3	−19.3	−5.9	0.4	1.0	−28.8	−7.2	−4.3	−1.4
89	−29.6	−9.9	−21.6	−6.9	−1.0	−0.2	−32.4	−8.1	−5.7	−2.5
90	−28.3	−8.4	−20.2	−5.6	−0.3	0.5	−29.8	−6.5	−4.8	−1.8
91	−29.7	−9.8	−21.7	−6.9	−1.1	−0.2	−32.5	−8.1	−5.6	−2.6
92	−28.1	−8.3	−20.0	−5.5	−0.2	0.6	−29.6	−6.4	−4.7	−1.7
93	−27.6	−8.6	−19.8	−5.6	0.4	1.2	−29.9	−6.8	−4.2	−1.3
94	−27.5	−8.6	−19.6	−5.5	0.5	1.2	−29.8	−6.8	−4.1	−1.4
95	−27.1	−6.7	−20.1	−4.4	0.7	1.5	−30.3	−5.4	−3.9	−1.1
96	−27.5	−7.6	−19.3	−4.7	0.4	1.3	−29.0	−5.7	−4.1	−1.0
97	−27.3	−6.6	−20.3	−4.4	0.7	1.5	−30.6	−5.2	−3.9	−1.0
98	−19.6	−4.7	−14.9	−3.2	5.2	6.1	−22.5	−4.7	1.3	3.8
99	−25.5	−6.8	−18.4	−4.2	1.0	1.9	−28.1	−5.5	−3.1	−0.5
100	−26.8	−7.6	−19.2	−4.7	1.3	2.1	−29.4	−6.0	−3.1	0.0
101	−23.1	−6.7	−17.0	−4.1	0.8	1.6	−25.6	−6.0	−3.3	−0.6
102	−27.8	−7.9	−19.6	−5.0	0.4	1.2	−29.5	−6.2	−3.9	−0.9
103	−27.2	−5.9	−20.0	−3.9	0.8	1.8	−30.2	−4.7	−3.6	−0.4
104	−27.6	−7.9	−19.4	−5.0	0.6	1.3	−29.4	−6.1	−3.9	−0.8
105	−26.4	−8.4	−18.7	−5.2	0.9	1.6	−28.3	−6.7	−3.5	−0.5
106	−26.7	−7.6	−19.0	−4.7	1.4	2.0	−29.3	−6.1	−3.0	−0.6
107	−42.7	−16.8	−30.2	−10.8	−7.0	−3.3	−69.3	−17.6	−15.0	−7.4
108	−39.9	−19.9	−27.9	−11.5	−7.0	−3.8	−64.7	−20.2	−14.0	−7.9
109	−43.6	−16.2	−31.2	−10.5	−7.4	−3.2	−70.8	−17.6	−15.2	−7.0
110	−40.2	−13.8	−28.8	−9.2	−6.6	−2.7	−65.2	−15.2	−13.9	−6.2
111	−40.3	−18.7	−28.7	−11.0	−7.2	−3.5	−66.2	−19.5	−14.1	−7.4
112	−43.9	−15.5	−31.4	−10.1	−7.3	−3.2	−71.5	−17.3	−15.0	−7.0

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Table 15 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
113	−40.1	−13.7	−28.6	−9.1	−6.5	−2.6	−65.2	−15.2	−13.6	−6.1
114	−40.7	−18.2	−29.2	−10.8	−7.2	−3.4	−67.1	−19.2	−14.1	−7.2
115	−43.6	−15.4	−31.2	−9.9	−7.2	−3.0	−71.4	−17.2	−14.8	−6.7
116	−40.5	−14.1	−29.1	−9.5	−6.8	−2.9	−65.9	−15.8	−14.3	−6.2
117	−40.8	−18.1	−29.3	−10.9	−7.3	−3.4	−67.3	−19.2	−14.1	−7.1
118	−40.2	−20.8	−34.3	−16.5	−9.6	−5.1	−55.1	−22.7	−12.4	−7.7
119	−34.4	−15.1	−29.0	−13.9	−9.5	−4.6	−48.8	−19.3	−11.4	−7.4
120	−39.6	−22.3	−34.5	−17.1	−9.4	−5.0	−54.1	−23.6	−12.0	−7.6
121	−36.3	−15.8	−29.7	−14.3	−9.6	−4.9	−50.6	−19.2	−12.0	−7.7
122	−39.0	−18.7	−33.6	−14.9	−9.0	−3.9	−55.4	−20.8	−11.5	−6.9
123	−36.0	−14.9	−30.4	−13.5	−9.6	−4.5	−50.4	−19.4	−11.5	−7.7
124	−41.3	−21.4	−35.8	−17.6	−10.4	−5.7	−58.5	−23.1	−13.2	−8.2
125	−37.0	−14.2	−30.7	−13.5	−9.8	−4.8	−51.0	−18.2	−12.0	−7.3
126	−36.2	−15.0	−30.0	−13.9	−9.8	−4.8	−50.2	−18.8	−11.8	−7.9
127	−41.9	−19.8	−35.3	−16.1	−9.9	−4.8	−58.3	−21.9	−12.3	−8.3
128	−55.8	−17.1	−35.3	−11.3	−11.4	−6.5	−60.0	−17.1	−14.5	−8.3
129	−53.7	−18.4	−33.9	−12.0	−11.9	−7.4	−56.8	−17.8	−14.6	−9.1
130	−54.8	−16.2	−35.2	−10.8	−11.0	−5.8	−59.5	−16.4	−13.6	−7.2
131	−52.4	−15.1	−34.0	−10.0	−10.5	−5.5	−56.8	−15.2	−13.0	−6.6
132	−53.4	−17.9	−34.1	−11.8	−11.7	−6.9	−56.9	−17.4	−14.1	−8.3
133	−57.0	−16.9	−37.1	−11.7	−12.3	−6.7	−62.1	−17.4	−14.8	−8.5
134	−52.7	−15.4	−34.3	−10.3	−11.0	−5.9	−57.0	−15.5	−12.7	−6.7
135	−53.8	−18.0	−34.9	−12.0	−12.3	−7.1	−57.9	−17.7	−14.2	−8.5
136	−56.8	−16.6	−36.8	−11.4	−12.0	−6.5	−61.9	−17.1	−14.8	−8.1
137	−52.9	−15.6	−34.6	−10.5	−11.2	−5.9	−57.5	−15.9	−12.9	−6.8
138	−53.9	−17.8	−35.0	−11.9	−12.3	−7.0	−58.1	−17.6	−14.4	−8.1
139	−37.7	−14.6	−26.3	−9.5	−6.7	−3.1	−62.4	−14.2	−12.4	−5.5
140	−39.0	−13.6	−27.6	−8.8	−7.1	−2.9	−64.6	−13.9	−12.5	−5.5
141	−35.5	−11.9	−25.0	−8.0	−6.4	−2.8	−59.1	−12.3	−11.5	−4.9
142	−56.2	−26.6	−44.1	−17.6	−3.6	−1.8	−58.1	−23.4	−13.8	−7.3
143	−52.8	−26.0	−41.5	−16.9	−3.0	−1.2	−53.2	−21.5	−13.2	−7.0
144	−52.4	−26.6	−41.7	−17.2	−3.3	−1.4	−53.0	−21.8	−13.0	−7.4

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Table 15 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
145	−55.7	−27.8	−43.0	−18.2	−4.1	−2.3	−56.9	−24.2	−13.5	−7.5
146	−52.3	−27.0	−40.6	−17.6	−3.5	−1.8	−52.4	−22.3	−13.0	−7.2
147	−53.3	−28.1	−41.2	−17.8	−3.7	−1.8	−53.0	−22.6	−12.8	−7.1
148	−17.8	−8.8	7.2	10.5	5.3	7.9	−71.7	−29.1	−17.2	−6.7
149	−25.6	−8.1	−0.6	4.6	−3.0	0.8	−97.9	−35.9	−28.4	−12.0
150	−43.0	−17.6	−33.8	−10.2	2.6	5.2	−46.9	−14.0	−5.7	−0.5
151	−33.2	−0.7	−32.4	−0.4	2.6	7.3	−43.9	−2.9	−5.0	3.3
152	−25.9	−10.1	−17.4	−2.7	−3.5	−0.1	−43.8	−11.8	−7.2	−3.2
153	−20.7	0.4	−17.6	−0.4	−3.1	1.5	−43.2	−8.8	−6.9	−1.4
154	−34.1	−17.6	−19.9	−6.2	−2.8	0.1	−51.1	−16.9	−9.6	−4.5
155	−32.6	−11.4	−23.6	−5.9	−4.7	−1.0	−49.4	−13.4	−8.8	−3.9
156	−26.7	−4.4	−17.7	−1.6	−3.0	1.0	−50.2	−8.3	−8.5	−1.5
157	−32.5	−9.2	−25.5	−7.1	−4.7	−0.4	−50.6	−13.4	−8.8	−3.6
158	−17.9	−8.9	6.8	10.2	5.7	8.3	−71.9	−29.1	−17.1	−6.3
159	−18.0	−8.8	6.7	10.2	5.6	8.1	−72.1	−29.2	−17.3	−6.7
160	−42.9	−17.5	−33.8	−10.2	3.0	5.6	−47.0	−14.1	−5.7	−0.3
161	−31.6	1.7	−31.0	1.7	4.7	9.3	−40.6	0.9	−3.2	5.7
162	−26.9	−13.1	−17.3	−3.1	−2.2	0.8	−41.0	−15.2	−6.8	−2.7
163	−24.5	−2.0	−19.0	−0.7	−3.2	1.8	−47.3	−8.0	−6.9	−1.2
164	−34.6	−18.0	−21.8	−7.1	−2.8	−0.4	−48.2	−17.3	−9.9	−5.0
165	−30.2	−15.9	−19.6	−5.4	−3.6	−0.7	−44.4	−16.6	−8.7	−5.5
166	−34.1	−7.7	−22.4	−4.6	−3.4	1.1	−59.0	−11.2	−10.2	−2.4
167	−37.1	−14.3	−26.6	−7.8	−5.5	−1.5	−54.5	−17.8	−9.9	−4.7
168	−18.0	−8.9	6.9	10.3	5.9	8.5	−72.1	−29.1	−16.9	−6.2
169	−18.1	−8.7	6.8	10.3	5.8	8.5	−72.7	−29.1	−17.4	−6.5
170	−43.4	−18.4	−34.0	−10.9	1.5	4.3	−46.8	−14.7	−7.0	−1.7
171	−46.6	−13.9	−40.4	−9.2	0.5	4.1	−54.9	−13.2	−8.8	−0.9
172	−27.7	−11.7	−16.4	−1.0	−3.1	0.8	−47.1	−13.8	−7.4	−3.0
173	−31.3	−6.4	−23.9	−3.2	−5.2	−0.4	−55.4	−10.5	−9.5	−3.3
174	−30.6	−16.7	−20.0	−5.8	−3.5	−0.7	−44.5	−17.0	−8.5	−5.4
175	−40.9	−12.3	−26.8	−6.6	−4.7	−0.2	−65.9	−14.2	−12.3	−3.8
176	−38.3	−13.2	−26.4	−7.5	−5.8	−0.8	−59.4	−13.0	−11.1	−3.8

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Table 15 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
177	−17.5	−8.4	7.3	10.7	6.3	9.0	−71.3	−28.7	−16.5	−5.5
178	−23.8	−1.8	1.0	7.3	−0.1	4.3	−100.0	−23.8	−24.9	−5.5
179	−43.2	−18.1	−33.8	−10.7	1.8	4.6	−46.6	−14.5	−6.5	−1.5
180	−43.9	−18.4	−34.9	−11.3	2.1	4.8	−48.1	−15.2	−6.8	−1.6
181	−32.7	−11.1	−22.3	−2.9	−5.2	−0.4	−55.5	−14.0	−9.1	−3.6
182	−32.8	−10.2	−22.8	−2.7	−5.3	−0.3	−56.1	−13.2	−9.2	−3.0
183	−33.6	−17.1	−20.9	−6.2	−1.9	0.5	−47.2	−16.7	−8.7	−3.8
184	−30.1	−16.3	−19.5	−5.4	−3.1	−0.2	−43.9	−16.5	−8.2	−4.1
185	−39.2	−13.9	−25.4	−6.2	−4.3	−0.1	−63.4	−15.0	−11.7	−3.8
186	−37.1	−16.1	−24.9	−7.3	−5.3	−1.0	−56.2	−14.9	−10.6	−4.0
187	−24.7	−8.0	3.7	8.9	2.9	6.6	−93.4	−30.6	−23.1	−7.0
188	−51.5	−16.4	−43.7	−11.4	−0.3	3.5	−60.5	−17.4	−9.9	−2.1
189	−37.3	−13.7	−25.6	−4.1	−6.9	−2.1	−61.6	−17.8	−11.8	−6.0
190	−46.4	−19.6	−31.2	−10.6	−7.8	−3.9	−72.2	−22.1	−16.3	−8.4
191	−43.0	−20.8	−30.0	−10.8	−8.1	−4.1	−64.0	−21.6	−14.5	−8.1
192	−25.3	−6.0	3.9	9.8	3.5	7.6	−97.3	−27.3	−23.1	−5.3
193	−53.4	−17.2	−46.0	−12.2	−1.2	2.7	−63.0	−17.8	−11.1	−2.5
194	−39.3	−14.1	−27.3	−4.5	−7.8	−2.5	−64.7	−18.4	−12.6	−6.4
195	−49.0	−20.5	−32.3	−11.1	−8.7	−4.5	−75.9	−22.9	−17.3	−9.0
196	−45.8	−22.1	−31.4	−11.4	−9.3	−5.0	−67.9	−22.3	−15.6	−8.7
197	−24.9	−5.3	3.3	8.9	3.7	7.6	−98.6	−21.0	−22.0	−4.1
198	−50.3	−9.4	−46.0	−9.2	−0.7	3.2	−60.0	−10.0	−10.1	−1.2
199	−36.5	−8.9	−29.4	−5.4	−6.9	−1.6	−62.6	−12.6	−11.4	−4.2
200	−44.1	−11.5	−31.9	−8.5	−7.2	−2.6	−72.7	−13.5	−15.0	−6.0
201	−46.9	−14.6	−36.1	−10.7	−8.6	−3.7	−66.5	−16.7	−13.8	−6.9
202	−22.4	−7.8	4.1	9.1	3.0	6.5	−83.3	−31.1	−22.4	−7.8
203	−52.9	−20.3	−44.2	−13.9	−1.5	1.9	−59.2	−18.6	−11.4	−4.0
204	−34.7	−15.8	−23.7	−5.6	−6.1	−2.2	−53.3	−19.3	−11.5	−6.7
205	−42.9	−21.5	−27.9	−10.5	−7.0	−3.7	−64.0	−22.5	−15.4	−8.9
206	−41.1	−23.6	−27.5	−11.6	−7.9	−4.7	−58.6	−23.0	−14.2	−8.9
207	−25.1	−7.7	2.6	7.6	2.0	5.6	−93.6	−23.2	−22.4	−6.5
208	−46.3	−9.8	−41.7	−9.4	−1.2	2.4	−53.1	−9.0	−9.7	−1.4

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Table 15 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
209	−34.9	−11.9	−26.1	−6.2	−7.7	−3.3	−58.1	−13.9	−11.4	−5.9
210	−41.4	−15.0	−29.2	−9.9	−7.6	−3.8	−66.1	−15.5	−14.7	−7.3
211	−34.5	−12.8	−25.8	−8.7	−6.9	−3.1	−53.0	−11.6	−11.8	−5.1
212	−22.1	−9.4	4.0	8.3	2.7	5.7	−81.7	−32.3	−22.0	−9.1
213	−49.4	−20.4	−40.8	−13.0	0.2	3.3	−55.1	−17.9	−9.4	−3.1
214	−35.1	−14.9	−21.8	−3.5	−5.3	−1.0	−56.5	−16.9	−10.2	−5.0
215	−40.8	−21.9	−24.9	−9.4	−4.7	−1.6	−61.2	−22.0	−12.3	−6.5
216	−40.9	−21.7	−26.9	−9.5	−7.1	−3.7	−57.5	−22.7	−12.9	−8.6
217	−23.8	−9.0	4.1	8.9	2.7	6.0	−89.0	−30.8	−22.8	−8.6
218	−53.9	−21.0	−45.3	−13.9	−1.5	2.0	−60.7	−18.7	−11.2	−4.1
219	−37.5	−15.0	−24.6	−4.3	−7.0	−2.4	−60.5	−17.3	−12.0	−6.5
220	−44.1	−21.1	−29.6	−10.0	−7.1	−3.9	−64.6	−22.7	−15.0	−8.7
221	−46.4	−22.0	−31.4	−10.5	−7.5	−3.5	−62.6	−22.8	−13.2	−9.0
222	−24.3	−2.8	2.9	8.7	3.5	7.4	−95.6	−14.4	−22.2	−3.9
223	−52.9	−20.2	−44.7	−13.5	−0.9	2.7	−60.3	−18.5	−10.5	−3.2
224	−37.5	−11.6	−29.6	−7.8	−7.8	−3.1	−62.1	−13.5	−12.3	−4.9
225	−40.5	−20.0	−26.5	−9.2	−5.1	−2.0	−59.3	−21.9	−13.1	−7.1
226	−44.0	−23.0	−30.3	−11.7	−8.4	−4.4	−64.6	−22.4	−14.8	−8.5
227	−23.4	−10.4	3.9	8.1	1.8	4.7	−86.8	−31.8	−22.9	−10.1
228	−44.6	−20.0	−36.8	−13.1	−0.4	2.2	−48.8	−16.9	−8.6	−3.6
229	−34.3	−15.8	−23.0	−5.8	−6.1	−2.9	−52.7	−18.0	−11.5	−6.9
230	−35.0	−17.7	−23.6	−8.6	−4.5	−2.3	−47.5	−18.2	−11.5	−6.0
231	−34.1	−20.7	−18.5	−7.1	−4.7	−1.6	−47.8	−17.8	−9.8	−5.0
232	−23.0	−9.5	4.2	8.4	2.5	5.4	−87.5	−30.6	−22.3	−9.0
233	−50.6	−19.0	−42.0	−12.4	−0.2	3.2	−56.8	−16.6	−9.3	−2.1
234	−35.2	−13.6	−22.5	−2.9	−5.9	−1.6	−58.1	−15.4	−10.2	−4.6
235	−43.0	−20.8	−29.4	−10.3	−5.3	−2.4	−62.7	−21.6	−13.0	−6.5
236	−37.0	−19.5	−24.6	−8.2	−6.7	−3.3	−51.7	−21.1	−11.7	−8.0
MAXD	−66.6	−28.1	−49.5	−18.2	−12.3	10.6	−100.0	−35.9	−28.4	−12.0
MD −36.4	−11.2	−23.0	−4.6	−2.9	0.9	−57.4	−14.8	−11.2	−3.7	
MAD	36.4	11.9	24.3	8.3	5.3	3.9	57.4	15.3	11.6	4.9

Table 16: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for HF. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	5.2	33.9	12.7	33.7	27.7	34.5	8.4	33.1	31.4	34.8
2	2.4	34.5	11.3	34.6	28.3	35.9	6.6	34.4	33.0	35.2
3	3.5	32.2	11.2	32.1	26.8	33.7	7.0	31.9	33.8	36.3
4	2.1	35.2	11.2	35.4	29.0	36.8	6.3	35.2	33.6	36.1
5	3.4	34.2	11.5	34.1	28.5	40.8	7.0	33.7	32.3	35.2
6	2.1	35.6	11.2	35.7	29.3	37.2	6.2	35.5	33.7	36.9
7	3.3	34.3	11.4	34.2	28.5	35.9	6.9	33.7	32.8	35.3
8	29.8	42.0	45.8	49.4	38.7	42.2	−29.5	24.8	23.7	35.8
9	29.8	42.7	46.6	50.5	40.1	43.8	−31.4	27.1	26.3	39.6
10	15.5	24.0	35.6	38.6	29.5	32.3	−38.2	7.1	14.1	24.3
11	16.8	25.7	36.4	39.5	30.6	33.4	−37.9	9.9	15.5	25.8
12	29.9	42.1	45.9	49.6	39.2	42.8	−29.8	25.1	25.0	36.4
13	31.2	44.1	48.0	52.0	41.6	45.4	−30.2	28.5	27.4	40.2
14	15.5	24.1	35.6	38.6	29.5	32.4	−38.3	7.2	14.6	24.4
15	18.9	29.2	38.8	42.2	33.3	36.3	−38.3	14.7	18.7	29.4
16	31.4	44.9	47.4	51.3	41.1	44.9	−30.5	27.5	26.0	39.0
17	31.3	44.4	48.1	52.3	41.9	45.7	−30.3	28.6	27.6	40.4
18	15.8	24.7	35.9	39.2	30.0	33.0	−38.2	7.9	15.2	25.1
19	19.5	30.4	39.5	43.0	34.0	37.2	−38.3	16.2	18.4	29.9
20	31.5	45.1	47.5	51.5	41.3	45.2	−30.7	27.6	26.5	39.1
21	40.6	56.1	43.4	56.3	54.8	57.2	39.8	56.8	54.3	56.9
22	24.5	35.5	28.7	39.6	40.8	42.4	25.8	39.5	39.2	41.7
23	40.0	56.6	43.1	57.2	55.7	57.9	39.8	57.7	54.0	57.2
24	38.1	54.2	41.1	54.8	52.8	54.8	37.7	55.3	51.6	54.6
25	40.3	57.1	43.6	57.6	55.9	58.1	39.8	58.0	54.4	57.5
26	38.8	54.2	41.9	54.8	53.1	55.2	38.5	55.2	52.1	55.1
27	40.3	55.6	42.9	55.7	54.6	57.0	39.2	56.1	53.7	56.6
28	40.8	56.4	43.5	56.5	55.0	57.3	40.0	57.0	53.9	56.7
29	40.5	57.2	43.5	57.8	56.3	58.6	40.2	58.3	54.8	58.2

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Table 16 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
30	40.8	59.3	44.5	59.6	57.3	59.7	40.6	60.0	56.6	59.7
31	31.5	45.1	35.5	48.0	49.0	50.8	32.2	48.2	47.6	50.1
32	41.6	60.0	45.2	60.4	58.5	60.8	41.1	60.9	57.3	60.7
33	41.3	56.9	43.9	57.1	55.5	58.0	40.1	57.3	54.0	57.7
34	40.9	56.5	43.5	56.5	55.1	57.5	39.9	56.9	54.2	57.0
35	41.7	58.6	44.7	59.2	57.7	60.0	41.3	59.6	55.8	59.3
36	43.9	62.7	47.5	63.1	61.1	64.8	43.4	63.5	60.1	62.9
37	42.4	58.1	45.0	58.3	56.7	59.2	41.3	58.4	55.1	58.6
38	21.0	41.6	24.4	39.5	37.4	43.7	1.5	37.1	37.8	42.5
39	24.1	45.7	29.1	45.1	41.5	48.2	2.3	42.5	41.8	47.4
40	21.0	41.6	24.5	39.8	37.8	44.3	1.1	37.2	38.1	43.4
41	25.1	47.8	30.2	47.4	43.8	50.7	2.6	44.5	43.9	50.2
42	21.3	42.0	24.7	40.1	38.3	44.9	1.0	37.3	38.8	44.2
43	25.9	49.0	30.9	48.5	44.8	51.8	3.1	45.5	45.0	51.5
44	20.9	41.7	24.3	39.8	38.1	44.7	0.6	36.9	38.6	44.1
45	37.1	56.6	39.1	58.3	54.8	64.5	26.1	54.0	60.4	63.6
46	9.9	21.7	11.2	25.4	29.9	35.0	3.5	20.4	32.0	34.0
47	22.3	36.2	22.4	35.1	34.2	41.9	14.0	32.6	38.5	42.0
48	39.2	61.7	42.0	64.1	59.1	70.3	27.9	59.5	66.3	70.1
49	14.8	31.3	18.1	35.5	37.3	44.0	8.9	30.6	40.5	43.5
50	23.0	38.2	23.8	37.4	36.5	44.7	13.6	34.9	41.2	44.3
51	34.5	53.4	36.9	54.9	52.7	62.4	24.4	50.8	58.4	61.6
52	40.7	64.4	43.8	66.8	61.5	73.3	29.5	62.3	68.8	72.7
53	17.1	34.7	20.5	38.8	40.5	47.8	10.8	34.2	44.3	46.8
54	23.4	39.3	24.5	38.5	37.6	47.6	13.9	36.0	42.6	45.9
55	36.5	55.3	38.5	56.4	53.6	63.2	26.8	52.3	59.5	60.7
56	12.3	36.6	21.7	37.3	28.3	35.8	11.3	34.2	32.7	36.3
57	10.5	39.0	21.8	40.2	30.1	38.8	10.7	36.9	35.0	39.7
58	11.6	36.0	21.0	36.7	27.8	35.7	10.7	33.6	31.7	35.9
59	14.0	41.2	22.6	40.3	30.7	39.5	11.7	37.6	34.9	40.1
60	11.5	35.8	20.7	36.4	27.8	35.7	10.4	33.3	31.8	36.1
61	11.2	41.5	23.0	42.7	31.9	41.4	11.2	39.4	41.2	45.3

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Table 16 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
62	11.3	35.6	20.6	36.3	27.6	35.6	10.2	33.1	31.9	36.1
63	26.5	48.3	31.0	48.0	44.3	51.2	6.0	46.7	44.9	50.9
64	−5.1	22.4	5.2	26.1	25.5	30.9	1.9	26.6	30.0	32.0
65	−5.6	18.1	4.1	22.5	22.6	27.5	1.9	23.3	24.1	25.3
66	−4.9	23.0	5.2	26.6	25.8	31.4	1.7	27.1	26.9	30.1
67	−3.9	22.2	4.8	25.3	24.0	29.4	2.4	25.9	25.1	27.4
68	−5.0	19.1	4.6	23.5	23.4	28.7	2.3	24.3	28.5	30.2
69	−5.4	22.9	4.4	26.3	25.4	31.2	0.8	26.7	27.1	28.5
70	−4.5	21.8	4.4	25.0	23.6	30.6	1.9	25.8	25.8	27.2
71	−5.3	18.9	4.0	23.2	23.0	28.5	1.6	23.8	27.5	29.5
72	−5.1	23.3	4.6	26.7	25.7	31.6	1.1	27.1	26.9	29.1
73	−4.4	21.9	4.4	25.1	23.7	29.4	1.7	25.6	26.2	27.0
74	−5.3	19.0	4.0	23.3	23.1	28.7	1.5	23.9	24.7	26.8
75	21.2	29.6	43.2	46.0	37.3	40.0	−35.6	13.6	22.0	31.4
76	22.2	31.8	43.4	46.6	38.0	41.0	−35.0	15.3	23.3	32.5
77	21.8	31.3	41.6	44.7	36.7	39.6	−33.5	15.9	22.0	31.6
78	21.2	29.8	42.8	45.8	37.3	40.0	−35.5	13.8	22.8	30.5
79	22.2	32.2	43.2	46.7	38.2	49.4	−35.2	15.8	23.0	32.8
80	22.7	32.4	42.3	45.6	37.5	40.5	−32.2	17.2	22.2	32.5
81	21.0	29.9	42.5	45.6	37.2	40.0	−35.7	13.9	22.1	31.9
82	22.7	32.8	43.7	47.2	38.7	41.8	−34.6	16.5	23.9	33.4
83	22.8	32.4	42.6	46.0	38.0	41.0	−33.0	16.7	22.7	32.3
84	21.6	30.5	43.0	46.1	37.8	40.7	−35.0	14.6	22.6	31.4
85	21.0	34.5	25.7	36.9	39.1	40.1	21.7	37.2	38.0	39.1
86	26.0	38.8	30.3	40.8	42.4	43.4	27.2	41.6	40.6	42.6
87	19.8	29.1	22.7	31.7	39.1	40.1	18.3	29.8	36.9	38.0
88	24.5	37.2	29.2	39.6	41.1	42.0	26.0	40.1	38.8	41.0
89	20.8	34.4	25.4	36.6	38.7	41.5	21.3	36.9	37.5	38.8
90	24.9	38.7	29.5	40.6	41.5	42.6	26.6	41.5	40.7	41.3
91	20.8	34.4	25.5	36.7	38.8	41.4	21.4	36.9	37.7	38.8
92	25.0	38.9	29.6	40.7	41.6	38.6	26.7	41.6	40.8	41.7
93	26.1	39.0	30.3	41.0	42.6	43.5	27.2	41.7	40.0	42.8

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Table 16 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
94	26.1	39.0	30.4	41.0	42.6	42.8	27.2	41.7	41.5	42.9
95	23.4	37.1	27.3	38.8	40.4	43.7	23.7	39.4	38.5	40.0
96	25.6	39.4	30.2	41.3	42.2	43.3	27.4	42.3	40.5	42.2
97	23.0	36.8	26.8	38.5	40.1	41.2	23.1	39.1	38.8	40.0
98	19.6	29.5	22.2	31.3	38.1	38.7	18.1	29.9	37.1	37.5
99	25.5	38.3	29.4	40.0	41.4	42.4	26.3	40.6	39.8	40.9
100	26.6	39.5	30.7	41.5	43.3	44.2	27.4	42.1	42.0	43.0
101	26.1	37.7	29.1	39.2	40.1	47.3	26.6	39.7	38.8	40.0
102	25.2	39.0	29.8	41.0	42.0	43.1	26.8	41.7	41.1	42.5
103	23.9	38.2	27.9	39.7	41.0	50.4	24.4	40.5	40.2	41.5
104	25.3	39.1	29.8	41.0	42.1	43.2	26.8	41.8	41.1	42.4
105	25.3	37.8	29.8	40.2	41.8	42.8	26.4	40.6	39.9	41.9
106	26.5	39.5	30.7	41.4	43.2	44.2	27.4	42.0	42.4	42.9
107	12.1	28.6	18.0	32.3	32.9	37.7	−6.6	28.0	32.3	36.9
108	9.7	22.3	15.2	27.4	28.8	33.0	−7.9	21.9	28.9	32.4
109	12.4	29.9	18.4	33.6	33.6	38.6	−6.7	29.0	33.9	37.6
110	11.7	28.7	17.0	31.3	30.9	35.6	−6.0	27.6	31.0	35.4
111	10.4	24.2	15.9	29.1	29.7	34.3	−8.0	23.7	30.3	33.7
112	12.7	30.9	18.8	34.5	34.1	39.3	−6.9	29.9	34.1	38.0
113	11.9	28.9	17.2	31.5	31.1	35.9	−5.8	27.9	31.2	35.8
114	10.7	25.2	16.2	29.8	30.4	35.2	−8.0	24.4	30.4	34.3
115	12.9	31.1	18.9	34.7	34.2	48.4	−6.8	30.0	35.1	38.6
116	11.8	28.9	17.0	31.5	31.0	35.9	−6.2	27.6	31.2	35.3
117	10.8	25.3	16.2	30.0	30.5	35.3	−7.9	24.6	30.6	34.3
118	17.1	30.3	19.3	34.0	36.5	42.3	9.9	30.1	39.1	41.5
119	17.7	28.2	17.2	27.8	28.7	34.6	8.8	25.2	32.3	33.7
120	15.9	28.0	17.6	31.9	35.4	41.1	9.7	28.1	38.3	39.8
121	17.7	28.6	17.9	28.6	29.8	35.6	9.1	26.3	32.9	35.0
122	19.2	32.4	21.0	35.8	37.5	43.9	10.3	32.1	41.8	43.2
123	18.5	30.1	18.1	29.8	30.0	36.6	10.0	27.0	34.1	35.7
124	17.6	30.6	18.9	33.7	36.4	42.5	8.4	30.4	39.6	41.4
125	20.0	32.5	20.0	31.7	31.8	38.2	11.7	29.6	35.6	37.6

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Table 16 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
126	18.0	29.2	17.9	28.8	29.7	35.9	9.8	26.6	33.2	35.4
127	19.6	33.7	21.5	37.0	38.8	45.5	10.7	33.3	42.4	45.1
128	2.3	24.3	14.3	28.2	23.6	29.6	4.0	25.3	27.6	31.5
129	0.9	20.7	12.9	25.3	21.0	26.4	3.5	22.6	24.9	27.9
130	3.3	25.0	14.3	28.5	24.0	30.4	4.3	25.8	28.8	31.6
131	2.9	24.0	13.2	27.2	22.4	28.5	4.0	24.8	27.1	29.8
132	1.6	21.5	13.3	26.0	21.5	27.4	3.9	23.3	26.2	28.7
133	2.7	25.5	14.4	29.1	24.0	30.7	3.8	26.2	27.8	31.9
134	2.5	23.7	12.9	26.8	21.9	28.2	3.8	24.6	26.8	29.5
135	1.6	21.8	13.1	26.2	21.5	27.7	3.6	23.4	25.5	29.1
136	3.0	25.8	14.7	29.4	24.2	31.1	4.1	26.6	28.8	32.3
137	2.7	23.9	13.0	27.0	22.1	28.5	3.8	24.7	27.1	29.8
138	1.8	22.2	13.3	26.5	21.7	28.0	3.7	23.7	26.1	29.2
139	11.5	26.4	17.1	30.3	31.7	36.3	−5.7	27.0	31.1	35.4
140	12.4	29.0	18.3	32.8	33.2	38.2	−5.6	29.2	32.9	37.0
141	11.3	26.9	16.4	29.7	29.9	34.4	−5.2	26.9	30.0	33.1
142	−6.5	11.8	0.3	18.3	26.5	28.5	−7.5	14.7	20.7	26.1
143	−7.5	9.2	−1.0	15.8	23.9	25.9	−7.0	13.4	17.9	23.2
144	−6.6	9.7	−0.6	16.4	24.1	26.3	−6.2	14.0	19.1	23.6
145	−3.4	13.5	3.8	20.3	27.6	29.7	−3.5	17.0	23.2	26.9
146	−4.6	10.9	2.3	17.8	25.1	27.1	−3.3	15.6	20.9	23.7
147	−4.0	11.7	3.0	19.1	26.0	28.1	−2.3	16.9	22.2	24.6
148	21.9	27.5	38.5	40.9	31.8	33.9	−23.5	7.9	17.6	25.2
149	23.2	34.1	39.6	43.1	32.4	35.6	−37.9	8.0	18.0	27.9
150	4.2	18.8	7.6	22.8	27.8	30.9	3.3	21.9	26.0	28.7
151	20.4	43.0	20.3	43.0	39.2	44.7	14.6	41.9	39.3	44.1
152	15.2	24.9	19.1	30.4	23.9	28.0	4.5	24.8	25.9	28.1
153	27.4	40.7	27.2	40.0	33.8	39.5	12.5	34.1	34.7	38.4
154	4.0	15.1	11.3	22.0	21.2	24.9	−8.3	15.5	19.5	22.9
155	12.8	26.1	16.4	29.8	25.9	30.6	2.6	25.4	26.9	30.1
156	15.2	30.3	19.4	31.7	27.0	31.9	−2.3	27.1	27.4	31.3
157	14.9	29.0	17.6	30.5	28.7	34.2	3.5	26.8	30.0	32.7

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Table 16 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
158	20.9	26.6	37.6	40.0	31.5	33.7	−24.4	7.2	17.5	25.0
159	21.2	27.0	37.9	40.3	31.8	33.9	−24.1	7.5	17.8	25.3
160	3.6	18.2	7.1	22.3	27.7	30.8	2.7	21.2	25.4	28.7
161	21.6	44.7	21.9	45.1	41.4	46.6	17.9	45.4	41.3	46.4
162	16.6	24.7	20.5	31.6	26.7	30.4	8.3	24.4	26.2	28.5
163	25.8	39.8	28.1	41.5	34.0	40.2	10.7	36.7	36.0	39.6
164	5.5	15.9	10.7	22.3	23.2	25.9	−3.9	16.5	21.0	23.6
165	15.3	24.4	19.7	31.1	27.6	31.3	7.5	25.6	27.9	29.2
166	13.7	31.0	19.6	32.7	30.7	36.3	−5.0	28.1	30.5	35.6
167	15.8	29.8	19.4	33.6	30.5	35.6	4.2	27.6	32.2	34.4
168	20.7	26.4	37.4	39.9	31.6	33.7	−24.8	6.9	16.9	24.8
169	21.1	27.0	37.9	40.4	32.0	34.1	−24.7	7.4	17.2	25.2
170	5.2	19.8	9.1	24.1	28.5	31.7	5.0	23.4	25.2	28.5
171	11.0	30.9	12.6	33.4	35.4	39.6	6.4	31.6	33.4	38.2
172	20.7	31.0	26.8	39.0	29.9	34.8	9.2	31.3	30.9	33.7
173	22.3	37.2	25.1	40.0	33.1	39.0	7.1	35.1	34.1	38.9
174	13.7	22.5	18.0	29.5	26.4	30.1	6.2	23.9	26.4	28.3
175	12.0	30.5	18.8	33.7	32.3	37.8	−6.1	29.0	31.1	36.4
176	18.9	34.9	24.0	38.7	35.2	41.4	5.2	36.4	36.6	38.9
177	21.1	26.7	37.8	40.2	31.9	34.1	−24.1	7.3	17.2	25.1
178	26.8	40.3	43.3	47.3	37.3	40.9	−36.6	20.2	21.1	34.7
179	5.3	19.9	9.2	24.2	28.7	31.9	5.1	23.5	25.1	28.6
180	2.4	17.0	5.9	21.2	26.7	29.8	1.3	19.9	23.8	27.4
181	25.6	38.8	30.4	44.9	36.0	42.0	11.7	38.2	37.9	41.3
182	26.5	40.3	31.1	46.0	37.0	43.2	12.3	39.6	39.2	42.6
183	5.8	16.1	11.0	22.6	23.6	26.3	−3.5	16.5	20.7	23.9
184	13.8	22.5	18.1	29.5	26.5	30.1	6.3	24.0	26.2	28.2
185	11.4	28.1	18.0	32.6	30.8	36.0	−6.0	27.3	29.8	34.3
186	15.9	29.6	20.9	35.3	31.5	37.0	3.8	31.9	32.9	36.5
187	27.9	38.2	47.6	50.9	41.4	44.5	−29.0	17.3	25.6	36.0
188	11.6	33.5	14.5	36.6	39.6	34.6	6.9	33.5	37.4	41.7
189	31.2	45.9	37.1	53.4	43.7	49.5	16.3	44.8	44.8	48.1

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Table 16 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
190	15.2	33.2	22.7	38.7	37.4	42.2	−3.4	31.4	36.3	40.8
191	20.3	35.0	25.6	41.6	38.3	43.1	6.8	35.7	40.6	43.2
192	29.1	40.9	49.3	53.2	43.6	47.1	−30.8	21.2	28.2	39.3
193	11.1	32.8	13.6	36.1	39.4	33.2	6.0	33.0	37.8	41.3
194	31.9	47.4	37.6	54.9	44.6	51.1	16.3	46.2	47.4	49.3
195	14.5	33.4	23.0	39.3	37.4	42.7	−4.8	31.7	37.6	41.4
196	20.1	35.8	26.4	43.0	38.4	44.0	5.9	37.1	42.4	44.4
197	25.0	36.3	46.6	50.2	41.4	44.7	−35.7	22.1	26.3	37.7
198	7.9	32.6	9.7	34.0	36.6	41.2	2.8	32.8	34.8	39.8
199	28.6	44.6	31.0	48.3	42.1	48.5	12.2	43.1	44.8	48.2
200	17.5	38.4	23.4	40.9	39.5	45.0	−3.0	37.1	39.1	44.5
201	20.6	39.7	24.7	43.0	40.6	46.7	7.9	39.2	44.6	45.6
202	26.8	36.0	45.7	48.9	39.4	42.3	−22.9	15.2	24.1	33.0
203	8.2	27.8	12.3	32.6	36.5	40.4	6.1	30.4	34.6	37.6
204	25.3	37.1	30.9	45.0	37.6	42.4	14.9	36.7	37.5	40.8
205	10.5	25.1	18.7	32.3	31.5	35.6	−3.9	24.8	30.7	34.1
206	16.3	28.1	22.6	35.9	33.1	37.2	5.8	30.2	33.9	35.9
207	24.5	34.6	45.7	48.9	39.7	42.7	−31.4	20.7	25.1	35.0
208	6.9	28.8	9.0	30.1	32.4	36.5	4.3	30.5	31.5	35.7
209	25.5	39.0	29.4	43.8	37.0	42.6	11.9	39.2	39.9	42.6
210	12.7	29.8	18.7	32.9	31.9	36.7	−4.4	29.7	32.4	37.1
211	16.8	30.8	20.5	34.0	31.4	36.4	5.5	33.4	35.7	38.0
212	25.2	33.0	43.5	46.3	37.1	39.5	−23.7	12.3	21.4	29.7
213	7.6	25.5	11.6	30.4	34.4	38.0	6.0	28.6	32.8	35.7
214	27.9	40.5	35.4	49.3	40.2	45.4	15.8	41.4	41.3	44.4
215	8.9	21.5	17.5	29.6	29.7	33.6	−5.3	22.0	29.7	32.3
216	16.9	29.2	24.3	37.8	33.2	37.6	7.9	30.7	34.3	35.7
217	26.7	35.6	46.3	49.6	39.9	42.6	−27.2	15.5	24.5	33.6
218	6.2	26.5	10.2	31.4	35.0	39.3	3.8	29.5	32.7	36.5
219	28.9	42.9	36.0	51.5	41.7	47.3	15.5	43.5	42.8	46.0
220	12.1	27.1	19.3	34.9	33.4	37.3	−1.3	26.8	32.3	35.3
221	17.0	32.0	24.3	40.0	36.5	41.6	7.9	33.2	38.0	40.0

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Table 16 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
222	25.6	38.1	46.9	50.4	41.9	45.0	−32.7	27.9	27.3	37.9
223	6.1	26.3	9.8	31.0	34.9	38.9	3.3	28.8	33.0	36.6
224	26.9	41.9	30.3	45.9	41.0	46.9	12.5	42.2	42.7	46.2
225	8.1	21.8	15.1	29.0	28.9	32.6	−4.7	21.0	27.1	30.3
226	16.5	30.3	23.0	38.4	35.6	40.4	4.1	32.8	38.4	40.4
227	25.6	33.3	44.6	47.4	37.6	40.0	−27.3	13.1	22.6	30.7
228	5.7	20.4	9.1	24.6	28.4	31.4	4.5	23.3	27.1	29.8
229	21.4	32.6	27.6	40.5	33.3	37.2	11.2	32.9	33.0	35.9
230	4.2	15.1	9.1	20.7	22.0	24.5	−4.8	14.8	20.5	23.3
231	13.5	23.1	22.9	32.3	27.6	31.6	5.9	27.6	28.7	30.0
232	25.1	33.0	44.2	47.0	37.5	40.0	−28.4	13.4	22.0	30.5
233	7.2	26.6	11.0	31.1	34.6	38.5	5.0	29.6	32.6	36.6
234	28.2	41.6	35.6	50.5	40.3	45.6	15.0	42.7	41.7	44.7
235	7.6	21.8	13.8	28.8	29.8	33.4	−5.7	21.7	29.1	32.6
236	15.8	27.0	22.1	34.9	29.8	34.0	7.7	28.1	30.8	32.2
MAXD	43.9	64.4	49.3	66.8	61.5	73.3	43.4	63.5	68.8	72.7
MD	17.5	33.4	25.1	38.2	35.4	39.9	2.7	30.7	33.5	37.8
MAD	18.2	33.4	25.1	38.2	35.4	39.9	15.4	30.7	33.5	37.8

Table 17: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the O3LYP functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−22.8	23.3	−10.1	23.9	21.8	28.4	−18.3	23.1	20.2	27.7
2	−28.0	23.9	−13.1	24.7	22.2	29.5	−22.0	24.6	20.4	28.7
3	−24.7	21.5	−12.0	22.1	20.8	27.5	−19.9	21.8	19.1	26.4
4	−28.5	25.1	−13.5	25.8	23.2	30.7	−22.7	25.7	21.3	30.1
5	−26.2	23.8	−12.7	24.3	22.5	29.7	−21.4	23.9	20.7	28.7
6	−28.5	25.6	−13.6	26.4	23.6	31.3	−22.9	26.2	21.8	30.5
7	−25.9	24.1	−12.4	24.5	22.9	30.0	−21.2	24.1	20.9	29.0

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Table 17 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
8	−10.2	9.7	12.4	18.7	10.8	15.5	−81.5	−10.8	−13.6	5.4
9	−9.1	12.1	14.1	20.7	12.8	17.8	−82.5	−6.7	−12.1	7.9
10	−22.2	−8.1	4.3	9.2	3.3	7.2	−84.9	−26.1	−21.0	−5.9
11	−19.0	−4.2	6.4	11.5	5.9	9.8	−83.5	−21.4	−18.4	−2.8
12	−9.3	10.7	13.2	19.5	11.8	16.7	−81.1	−9.8	−12.5	6.4
13	−7.3	14.2	15.8	22.7	14.6	19.8	−81.0	−4.9	−10.3	10.1
14	−21.7	−7.5	4.6	9.6	3.6	7.6	−84.6	−25.7	−20.5	−5.5
15	−16.5	0.7	9.4	14.9	9.1	13.3	−83.7	−14.9	−15.9	1.5
16	−6.5	15.5	16.0	22.9	15.1	20.3	−80.5	−4.9	−9.9	10.6
17	−6.8	14.8	16.3	23.4	15.2	20.4	−80.8	−4.3	−9.8	10.9
18	−21.1	−6.3	5.3	10.7	4.4	8.5	−84.3	−24.5	−19.9	−4.0
19	−15.6	2.4	10.3	16.2	9.9	14.4	−83.5	−12.8	−15.2	2.9
20	−6.0	16.1	16.5	23.4	15.6	20.8	−80.3	−4.4	−9.3	11.3
21	11.3	31.9	15.7	32.2	34.4	36.5	7.8	31.5	30.2	34.6
22	−8.0	6.4	−1.5	12.1	17.5	18.9	−8.6	10.1	13.2	16.1
23	12.1	33.3	16.5	33.9	36.4	38.5	9.1	32.7	31.8	36.2
24	10.0	31.2	14.6	31.9	34.0	35.9	6.7	30.8	29.5	33.8
25	10.1	32.4	15.0	33.0	35.0	37.1	6.5	31.8	30.6	35.1
26	10.3	30.5	14.6	31.0	33.4	35.4	7.0	29.9	29.2	33.3
27	11.3	31.9	15.5	32.0	34.5	36.6	7.6	31.1	30.3	34.7
28	13.5	34.1	17.6	34.1	36.1	38.3	10.1	33.5	32.1	36.4
29	12.7	34.2	17.1	34.6	37.1	39.2	9.7	33.5	32.5	37.0
30	12.5	36.2	17.6	36.2	37.9	40.2	9.5	35.3	33.5	38.1
31	0.4	18.8	6.6	22.5	27.4	29.0	−0.9	21.4	22.6	26.2
32	12.0	36.3	17.1	36.5	38.2	40.5	8.6	35.6	33.7	38.6
33	14.4	35.1	18.4	35.0	37.0	39.5	10.9	34.0	33.2	37.7
34	14.3	35.0	18.3	34.9	36.8	39.1	10.8	34.1	32.8	36.9
35	14.1	35.8	18.5	36.2	38.6	40.8	10.9	35.0	33.9	38.5
36	14.5	39.4	19.6	39.5	41.0	43.3	11.0	38.6	36.4	41.4
37	16.0	36.7	19.9	36.6	38.6	41.1	12.5	35.5	34.8	39.2
38	2.1	33.0	10.5	31.6	31.4	37.3	−23.5	27.7	24.7	34.5
39	2.0	34.4	12.5	34.3	32.5	38.9	−26.8	30.4	25.6	36.4

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Table 17 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
40	2.3	33.5	10.8	32.2	32.2	38.4	−23.8	28.0	25.7	35.5
41	2.2	36.5	13.1	36.5	34.5	41.1	−27.6	32.4	27.2	38.3
42	3.1	34.3	11.4	32.9	33.0	39.3	−23.6	28.5	26.6	36.6
43	3.0	37.9	13.8	37.8	35.5	42.3	−27.2	33.6	28.4	40.1
44	3.0	34.3	11.2	32.8	33.0	39.3	−23.7	28.4	26.6	36.6
45	8.9	38.7	16.4	41.1	41.7	50.5	−8.1	34.6	41.0	47.5
46	−15.3	−0.3	−10.2	6.2	14.6	19.0	−28.2	−2.1	11.6	15.8
47	1.2	25.2	8.1	26.4	28.4	35.3	−11.5	21.0	27.4	32.7
48	8.8	43.3	17.5	46.4	45.6	55.9	−8.8	39.5	45.6	52.0
49	−14.2	9.4	−6.1	15.8	22.3	28.2	−26.4	7.9	19.8	24.9
50	−0.3	26.4	8.1	27.8	29.7	37.3	−14.5	22.5	28.8	34.6
51	8.3	37.8	16.4	40.0	41.5	50.1	−7.6	33.8	40.7	47.1
52	9.7	46.1	18.9	49.2	47.8	58.7	−7.6	42.4	48.2	56.0
53	−12.7	13.2	−4.1	19.0	25.2	31.8	−25.6	11.7	22.7	28.3
54	−0.3	27.9	8.8	29.2	31.1	38.8	−14.4	24.0	30.0	35.9
55	9.9	39.8	17.9	41.6	42.2	50.9	−5.1	35.2	41.8	48.2
56	−14.3	26.6	1.7	28.0	22.5	29.5	−21.8	22.1	20.4	28.3
57	−18.8	28.9	−0.4	30.7	23.9	32.0	−26.0	24.8	21.9	30.4
58	−14.3	26.6	1.4	27.8	22.4	29.7	−21.8	22.1	20.5	28.3
59	−15.6	30.1	0.3	30.2	23.3	31.4	−25.2	24.6	21.5	30.1
60	−14.2	26.7	1.3	27.8	22.5	30.0	−21.9	22.0	20.6	28.5
61	−19.0	31.8	−0.2	33.4	26.0	34.7	−26.7	27.6	24.0	33.3
62	−14.1	26.8	1.5	27.9	22.6	30.0	−21.9	22.0	20.7	28.5
63	11.8	43.6	20.6	42.5	39.0	45.4	−15.9	41.1	34.3	44.5
64	−44.1	2.4	−27.2	8.2	12.8	18.0	−35.0	8.3	9.6	16.4
65	−43.5	−3.1	−28.0	3.4	8.8	13.6	−33.9	3.8	6.1	12.1
66	−43.1	4.0	−26.8	9.4	13.7	19.2	−34.8	9.5	10.4	17.7
67	−42.0	1.9	−27.2	7.3	10.8	16.1	−34.2	7.4	8.2	15.0
68	−42.9	−1.8	−27.5	4.6	9.8	15.0	−33.7	4.8	7.3	13.6
69	−43.3	4.7	−27.4	9.8	13.8	19.5	−35.5	9.8	10.4	18.1
70	−42.6	1.9	−27.7	7.2	10.6	16.2	−34.9	7.3	7.9	14.7
71	−42.6	−1.4	−27.7	4.8	9.8	15.1	−34.1	4.9	7.0	13.7

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Table 17 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
72	−42.6	5.3	−26.9	10.4	14.3	20.1	−35.0	10.3	10.9	18.9
73	−42.0	2.4	−27.3	7.7	11.0	16.6	−34.6	7.6	8.5	15.5
74	−42.6	−1.2	−27.7	5.1	9.9	15.4	−34.1	5.1	7.3	14.1
75	−18.7	−4.1	8.0	12.8	7.7	11.5	−87.0	−23.2	−17.0	−2.2
76	−15.6	0.8	10.2	15.8	10.3	14.5	−84.6	−19.1	−14.4	1.6
77	−17.1	−0.8	7.6	13.1	7.8	12.0	−83.9	−19.4	−16.3	−0.8
78	−17.4	−2.5	8.8	13.7	8.7	12.5	−85.6	−21.9	−15.7	−0.8
79	−15.1	2.1	10.6	16.7	10.9	15.3	−84.4	−17.7	−14.3	2.9
80	−15.6	0.9	8.9	14.4	9.1	13.2	−82.3	−17.7	−15.1	1.2
81	−17.1	−1.7	8.9	14.3	8.9	13.0	−85.4	−21.0	−15.7	−0.2
82	−14.2	3.0	11.4	17.5	11.7	16.1	−83.5	−16.7	−13.4	3.7
83	−15.5	1.0	9.2	15.1	9.6	13.7	−83.0	−18.1	−14.9	1.7
84	−16.1	−0.7	9.8	15.2	9.8	13.9	−84.4	−20.0	−14.7	1.1
85	−9.4	9.6	−2.9	12.4	18.4	19.2	−12.2	11.3	12.9	16.3
86	−4.7	13.8	1.5	16.3	22.2	23.1	−6.9	15.4	16.9	20.2
87	−0.2	13.6	3.8	15.7	24.8	25.6	−2.9	13.7	19.7	22.8
88	−4.8	12.6	1.3	15.3	21.5	22.2	−6.4	14.2	16.1	19.5
89	−8.7	10.5	−2.5	12.9	18.6	19.5	−11.7	11.7	13.2	16.6
90	−4.5	14.8	1.7	16.9	22.0	22.9	−6.2	16.3	16.7	20.1
91	−8.8	10.5	−2.6	12.9	18.5	19.5	−11.8	11.8	13.2	16.6
92	−4.3	14.9	1.8	17.0	22.1	23.1	−6.1	16.4	16.8	20.3
93	−3.8	14.7	2.1	17.0	22.9	23.8	−6.2	16.1	17.6	21.2
94	−3.7	14.8	2.3	17.0	23.1	23.8	−6.1	16.1	17.6	21.2
95	−5.1	15.0	0.4	16.8	21.7	22.6	−8.4	15.8	15.7	19.7
96	−3.4	16.0	2.8	18.1	23.0	24.0	−5.1	17.4	17.5	21.6
97	−4.9	15.5	0.5	17.3	22.0	23.0	−8.3	16.4	16.0	20.3
98	1.7	16.1	5.2	17.2	25.5	26.5	−1.1	15.9	20.7	23.7
99	−2.4	16.0	3.0	17.9	23.0	24.0	−5.1	16.8	17.6	21.2
100	−2.6	16.1	3.2	18.3	24.2	25.1	−5.3	17.4	18.5	22.5
101	1.0	17.1	5.3	18.9	23.7	24.6	−1.7	17.5	18.4	22.2
102	−3.5	15.9	2.7	18.0	23.1	24.1	−5.4	17.1	17.6	21.4
103	−3.8	17.2	1.8	18.7	23.1	24.2	−6.9	17.9	17.3	21.7

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Table 17 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
104	−3.3	15.9	2.9	18.0	23.3	24.1	−5.3	17.1	17.6	21.3
105	−2.2	15.2	3.6	17.7	23.6	24.5	−4.2	16.5	18.1	21.8
106	−2.3	16.3	3.5	18.4	24.4	25.2	−5.0	17.4	18.8	22.6
107	−14.3	11.2	−2.3	17.2	20.2	24.7	−40.5	9.9	11.9	20.8
108	−19.0	0.4	−7.3	9.2	13.0	16.7	−43.3	−0.3	5.3	12.4
109	−13.2	14.0	−1.3	19.6	21.8	26.7	−39.9	12.1	13.7	22.8
110	−13.5	12.9	−2.5	17.5	19.1	23.7	−38.0	11.0	11.3	20.1
111	−16.7	4.4	−5.4	12.4	15.4	19.6	−42.1	3.3	8.0	15.6
112	−12.0	16.1	0.0	21.6	23.3	28.3	−39.1	14.0	14.8	24.7
113	−12.9	13.4	−1.9	17.9	19.5	24.2	−37.5	11.5	11.7	20.9
114	−16.0	6.2	−4.8	13.8	16.6	21.0	−41.8	4.8	8.7	16.9
115	−11.5	16.5	0.4	22.0	23.7	28.6	−38.7	14.3	15.2	24.9
116	−12.5	13.7	−1.7	18.3	19.9	24.5	−37.5	11.6	11.9	20.8
117	−15.8	6.6	−4.6	14.1	16.7	21.3	−41.7	5.1	9.0	17.6
118	−7.1	12.9	−1.7	17.0	23.9	29.0	−21.5	10.7	20.7	25.4
119	−4.2	15.3	0.4	16.4	20.3	25.8	−18.2	11.0	18.6	22.9
120	−10.2	7.7	−5.4	12.8	20.7	25.7	−24.0	6.1	17.6	22.1
121	−5.5	15.2	0.3	16.6	20.9	26.2	−19.4	11.7	18.8	22.9
122	−3.7	17.1	1.1	20.6	26.4	32.2	−19.6	14.8	23.7	28.6
123	−5.0	16.5	−0.2	17.8	21.2	27.1	−19.1	11.8	19.7	24.3
124	−6.9	13.5	−1.9	17.1	24.2	29.6	−23.4	11.6	21.0	25.8
125	−3.9	19.4	1.7	20.0	23.2	28.9	−17.5	15.2	21.1	25.9
126	−4.8	16.7	0.6	17.7	21.3	27.1	−18.4	12.7	19.6	23.7
127	−4.3	18.3	1.6	21.8	27.8	33.7	−20.1	16.0	24.7	30.3
128	−31.6	7.3	−11.7	13.2	12.5	18.0	−36.4	6.8	8.8	15.9
129	−32.4	3.0	−13.3	9.4	8.9	14.0	−36.3	3.2	5.8	12.1
130	−30.4	8.4	−11.5	13.9	12.9	18.9	−35.8	7.6	9.8	17.2
131	−30.7	6.8	−12.8	12.1	11.0	16.7	−35.6	6.3	8.2	15.4
132	−31.3	4.4	−12.6	10.6	9.9	15.4	−35.5	4.4	7.2	13.7
133	−30.5	10.0	−11.3	15.2	13.8	20.1	−36.2	9.0	10.3	18.2
134	−30.7	6.8	−12.9	12.1	10.7	16.6	−35.6	6.3	8.0	15.4
135	−30.9	5.1	−12.6	11.2	10.1	16.0	−35.6	4.9	7.3	14.3

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Table 17 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
136	−30.0	10.5	−10.7	15.7	14.2	20.6	−35.8	9.4	10.9	18.9
137	−30.2	7.4	−12.5	12.6	11.2	17.2	−35.3	6.7	8.5	16.0
138	−30.5	5.9	−12.3	11.8	10.6	16.6	−35.4	5.6	7.9	14.8
139	−7.4	15.3	3.4	20.3	22.3	26.5	−31.6	15.2	16.2	24.1
140	−5.0	20.1	5.6	24.7	25.4	30.2	−30.1	19.3	19.2	28.0
141	−6.0	17.3	3.7	21.0	21.6	25.8	−29.2	16.5	15.8	23.8
142	−44.2	−14.7	−33.3	−5.9	7.6	9.7	−46.4	−12.0	−3.7	3.7
143	−42.8	−16.0	−32.6	−7.1	6.3	8.5	−43.5	−11.8	−4.8	1.9
144	−41.6	−15.9	−32.0	−6.7	6.9	9.1	−42.4	−11.4	−4.0	2.8
145	−43.9	−16.0	−32.6	−6.8	7.0	9.1	−45.5	−12.9	−3.5	3.5
146	−42.5	−17.1	−32.1	−8.1	5.8	7.7	−42.9	−12.9	−4.8	1.6
147	−42.7	−17.5	−31.8	−7.6	6.4	8.6	−42.5	−12.3	−3.9	2.5
148	−20.6	−11.7	2.6	6.1	0.8	3.8	−73.3	−32.5	−21.6	−11.0
149	−23.5	−6.2	0.3	5.9	−1.8	2.6	−94.2	−34.0	−26.6	−9.8
150	−39.3	−14.2	−30.9	−6.5	5.9	9.0	−42.7	−10.3	−4.2	2.4
151	−11.6	21.0	−11.6	21.4	24.0	29.8	−21.8	18.9	15.9	25.7
152	−13.2	2.4	−5.1	10.2	8.6	12.6	−30.5	0.8	4.2	9.4
153	2.2	23.4	5.1	23.0	19.9	25.2	−19.5	14.6	15.8	22.2
154	−22.6	−6.5	−8.4	5.5	8.1	11.5	−38.8	−5.7	0.3	6.4
155	−11.8	9.4	−2.8	15.4	16.3	20.6	−27.8	7.8	11.6	17.2
156	−2.3	19.9	6.7	23.0	20.9	25.7	−25.0	16.1	15.2	22.8
157	−8.0	15.3	−1.1	18.0	20.1	25.1	−25.4	11.4	15.4	21.6
158	−20.3	−11.3	2.7	6.2	1.6	4.6	−73.1	−32.1	−20.8	−10.1
159	−20.4	−11.4	2.5	6.1	1.4	4.4	−73.4	−32.3	−21.0	−10.3
160	−38.8	−13.7	−30.6	−6.2	6.5	9.7	−42.4	−10.1	−3.7	2.8
161	−9.1	24.3	−9.5	24.4	26.8	32.4	−17.7	23.7	18.4	28.6
162	−18.1	−4.6	−9.0	5.8	6.3	9.8	−31.6	−6.4	0.7	5.2
163	1.6	24.0	6.4	25.3	22.2	28.2	−20.6	18.2	18.6	25.6
164	−25.7	−9.5	−13.0	2.0	5.7	8.5	−38.6	−8.6	−2.2	3.2
165	−19.3	−5.0	−8.8	5.8	7.2	10.6	−32.8	−5.5	1.1	5.8
166	−7.4	18.6	4.3	22.3	22.8	28.0	−31.5	15.2	15.7	24.8
167	−15.6	7.2	−5.3	14.2	16.1	20.7	−32.4	4.0	10.9	16.7

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Table 17 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
168	−20.1	−11.1	2.9	6.5	2.0	5.1	−73.0	−31.9	−20.4	−9.7
169	−20.0	−10.8	3.0	6.7	2.1	5.2	−73.5	−31.7	−20.4	−9.4
170	−39.8	−14.9	−31.3	−7.3	4.6	7.9	−42.7	−11.0	−5.4	1.1
171	−36.4	−3.9	−31.0	1.2	10.2	14.6	−44.1	−3.0	−0.4	8.9
172	−13.1	2.6	−2.2	13.7	10.7	15.2	−31.7	0.8	5.5	11.0
173	−5.1	19.8	1.8	23.2	20.5	26.3	−28.4	15.8	15.9	23.5
174	−20.1	−6.3	−9.7	4.9	6.7	10.1	−33.4	−6.4	1.0	5.4
175	−16.0	12.4	−1.8	18.7	19.7	25.0	−40.1	10.5	11.8	21.4
176	−11.3	13.7	0.3	19.5	20.6	26.3	−31.9	13.8	15.3	23.4
177	−19.6	−10.6	3.3	6.9	2.4	5.5	−72.2	−31.4	−20.0	−9.1
178	−15.8	6.0	7.7	14.5	6.8	11.9	−90.5	−16.5	−18.4	1.6
179	−39.5	−14.6	−31.0	−7.0	4.9	8.2	−42.4	−10.7	−5.1	1.4
180	−39.5	−14.3	−31.3	−6.9	6.0	9.2	−43.2	−10.9	−4.3	2.3
181	−11.4	10.0	−1.5	18.6	15.3	21.0	−33.3	7.4	10.6	17.5
182	−10.0	12.4	−0.4	20.3	16.8	22.7	−32.3	9.7	12.3	19.5
183	−24.5	−8.4	−11.9	3.0	6.7	9.6	−37.4	−7.8	−1.1	4.5
184	−19.6	−5.8	−9.2	5.3	7.1	10.5	−32.7	−5.9	1.4	5.8
185	−16.6	8.4	−2.8	16.7	17.6	22.5	−39.9	7.3	9.7	18.7
186	−15.6	5.2	−3.8	14.1	15.4	20.4	−34.2	6.3	9.8	17.1
187	−19.9	−2.9	6.4	12.0	5.6	9.9	−87.4	−26.5	−20.1	−3.8
188	−36.7	−1.2	−30.2	3.3	13.4	18.0	−45.6	−2.6	2.3	11.3
189	−13.1	10.9	−2.3	20.0	16.3	22.0	−37.0	6.4	10.7	17.9
190	−20.2	6.7	−5.5	15.5	17.4	22.0	−45.7	3.8	8.3	17.3
191	−18.5	3.9	−6.2	13.5	15.5	20.2	−39.3	2.6	8.5	16.0
192	−18.2	1.4	8.9	15.3	8.4	13.3	−89.0	−20.8	−17.8	0.3
193	−37.8	−1.2	−31.7	3.4	13.3	18.1	−47.4	−2.3	2.1	11.6
194	−12.8	12.7	−1.7	22.0	17.5	23.8	−37.7	8.1	12.0	19.7
195	−21.0	7.5	−4.9	16.7	17.9	23.1	−47.6	4.6	8.9	18.5
196	−19.6	4.4	−6.0	14.6	15.8	21.0	−41.5	3.7	9.1	16.9
197	−12.1	7.2	14.0	20.2	14.5	19.0	−84.5	−9.7	−11.2	7.1
198	−27.4	13.6	−24.4	13.6	21.3	26.0	−36.8	12.7	10.9	21.4
199	−3.6	24.0	2.5	27.4	24.9	31.1	−29.2	20.1	20.2	28.4

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Table 17 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
200	−7.5	25.0	4.0	27.9	28.3	33.7	−35.6	22.6	20.1	30.5
201	−11.0	21.5	−1.0	25.3	26.8	32.5	−30.3	19.1	21.2	29.1
202	−20.3	−5.3	4.2	9.5	3.0	7.1	−80.2	−29.5	−21.6	−6.8
203	−42.3	−9.6	−35.1	−3.7	8.0	12.0	−48.7	−8.4	−3.2	5.4
204	−18.2	1.0	−8.0	10.8	9.7	14.3	−36.4	−2.8	3.7	9.5
205	−23.9	−2.5	−9.3	8.3	11.0	14.9	−44.7	−4.0	2.3	9.5
206	−23.1	−5.6	−10.3	5.9	9.0	12.8	−40.6	−5.5	2.3	8.5
207	−16.9	0.3	8.9	14.3	8.1	12.2	−84.2	−16.5	−16.2	0.1
208	−27.6	8.9	−24.3	9.0	16.5	20.8	−34.1	9.7	7.1	16.3
209	−8.2	14.6	−0.4	20.1	17.8	23.0	−30.8	12.4	13.4	20.2
210	−13.7	12.3	−2.1	17.4	18.8	23.2	−37.9	11.5	11.4	19.9
211	−7.4	14.3	0.5	18.0	19.3	23.7	−25.5	15.3	14.2	21.3
212	−21.8	−8.9	2.1	6.8	1.0	4.4	−80.4	−32.6	−23.3	−10.2
213	−42.3	−13.3	−35.1	−6.4	6.2	9.8	−47.9	−11.1	−4.8	2.8
214	−16.5	3.7	−4.0	14.9	12.3	17.3	−37.4	1.6	6.8	13.0
215	−26.0	−7.5	−10.6	5.1	8.9	12.6	−46.0	−7.8	0.9	7.2
216	−24.4	−5.0	−10.9	7.1	8.9	12.8	−40.7	−6.3	2.6	7.7
217	−21.2	−6.2	4.5	9.7	3.1	6.9	−85.1	−28.9	−21.9	−7.4
218	−44.0	−11.1	−36.8	−4.5	7.1	11.4	−50.7	−9.1	−4.2	4.3
219	−15.1	7.5	−3.2	17.9	14.3	19.7	−37.5	5.1	8.6	15.5
220	−23.8	−0.7	−9.7	10.3	12.3	16.2	−43.7	−2.7	3.6	11.2
221	−25.5	−0.8	−11.0	10.6	13.0	17.6	−41.4	−1.9	6.7	12.7
222	−10.9	10.2	14.4	20.6	15.0	19.4	−81.0	−2.5	−10.8	8.1
223	−42.6	−9.8	−35.8	−3.7	8.1	12.5	−49.8	−8.5	−3.0	5.7
224	−8.0	17.8	−0.9	21.6	20.8	26.4	−32.0	15.7	15.6	23.6
225	−23.5	−3.0	−10.1	7.7	10.9	14.5	−41.9	−5.1	2.4	9.1
226	−20.9	0.3	−7.9	11.2	13.7	18.4	−41.2	0.5	6.9	14.2
227	−22.9	−9.9	2.1	6.5	0.0	3.3	−85.1	−32.2	−24.2	−11.3
228	−39.1	−14.6	−32.4	−7.9	4.4	7.5	−43.0	−11.4	−5.1	1.1
229	−20.5	−1.9	−9.8	8.0	7.2	10.9	−38.4	−4.2	0.8	6.7
230	−25.7	−8.4	−14.6	0.8	4.3	6.9	−37.9	−9.2	−3.3	2.4
231	−23.3	−10.2	−8.7	2.8	4.7	8.3	−37.0	−7.6	−0.8	4.2

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Table 17 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
232	−20.9	−7.5	4.0	8.5	2.2	5.7	−84.2	−29.5	−22.1	−8.6
233	−40.8	−9.2	−33.4	−2.9	8.6	12.6	−46.7	−6.9	−2.0	5.7
234	−14.1	7.4	−2.3	18.0	14.1	19.2	−36.4	5.6	8.6	15.3
235	−26.0	−4.0	−12.6	6.7	11.0	14.4	−45.0	−4.9	2.6	9.8
236	−23.0	−5.3	−11.2	5.9	6.8	10.7	−37.6	−7.2	1.2	5.7
MAXD	−44.2	46.1	−36.8	49.2	47.8	58.7	−94.2	42.4	48.2	56.0
MD	−15.3	9.9	−2.9	16.2	17.4	21.8	−35.8	5.9	8.7	16.9
MAD	17.6	14.1	10.7	17.1	17.4	21.8	37.0	15.6	15.2	18.1

Table 18: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the PBE0 functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−21.7	18.3	−11.7	17.3	14.4	20.4	−18.1	17.8	14.1	20.2
2	−26.8	18.2	−14.9	17.5	14.2	20.9	−21.9	18.6	13.9	20.2
3	−23.6	16.5	−13.5	15.7	13.5	19.6	−19.8	16.4	13.1	19.1
4	−27.4	19.1	−15.3	18.4	15.0	21.9	−22.5	19.5	14.5	21.3
5	−25.0	18.3	−14.4	17.3	14.8	21.3	−21.2	18.1	14.3	20.7
6	−27.4	19.6	−15.5	18.8	15.4	22.4	−22.8	19.9	14.8	21.8
7	−24.8	18.6	−14.1	17.5	15.2	21.6	−21.1	18.2	14.8	20.9
8	−9.7	6.6	9.5	14.3	5.7	10.0	−75.6	−12.8	−13.7	1.6
9	−9.4	7.9	10.3	15.4	6.9	11.4	−77.3	−9.8	−13.3	3.1
10	−20.3	−8.7	3.8	7.6	0.5	4.0	−78.8	−26.3	−19.4	−6.9
11	−17.9	−5.7	5.1	9.0	2.4	5.8	−77.8	−22.4	−17.7	−4.9
12	−9.2	7.3	9.9	14.8	6.5	10.9	−75.5	−12.2	−13.1	2.2
13	−7.8	9.8	11.9	17.2	8.6	13.3	−76.0	−8.2	−11.3	5.1
14	−19.9	−8.2	4.1	8.0	0.8	4.3	−78.6	−26.0	−19.3	−6.8
15	−16.4	−2.3	6.8	11.2	4.4	8.1	−78.7	−17.4	−15.8	−1.9
16	−7.0	11.0	12.0	17.3	9.1	13.7	−75.2	−8.2	−11.0	5.8
17	−7.4	10.2	12.2	17.7	9.1	13.7	−75.8	−7.8	−11.0	5.7

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Table 18 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
18	−19.4	−7.3	4.5	8.8	1.4	5.1	−78.3	−25.0	−18.2	−5.3
19	−15.8	−1.1	7.4	11.9	4.9	8.8	−78.8	−15.8	−15.4	−1.6
20	−6.6	11.5	12.4	17.7	9.5	14.2	−75.3	−7.8	−10.1	6.3
21	6.2	23.7	9.3	23.3	24.1	26.4	3.6	23.7	22.3	25.5
22	−9.5	3.0	−3.7	7.9	11.5	13.0	−9.2	6.9	9.4	11.8
23	6.3	24.5	9.4	24.3	25.5	27.7	4.0	24.3	23.0	26.5
24	4.7	22.8	8.1	22.8	23.5	25.4	2.2	22.7	21.2	24.5
25	4.7	23.7	8.3	23.5	24.3	26.5	2.0	23.5	22.0	25.3
26	5.2	22.5	8.4	22.4	23.4	25.5	2.8	22.3	21.2	24.2
27	6.2	23.6	9.1	23.0	24.3	26.5	3.3	23.2	22.3	25.2
28	7.9	25.4	10.8	24.8	25.5	27.9	5.4	25.2	23.6	26.7
29	6.7	25.1	9.8	24.8	26.0	28.2	4.4	24.9	23.3	26.8
30	6.2	26.5	10.0	25.8	26.4	28.7	4.0	26.1	24.0	27.5
31	−3.3	12.4	1.9	15.4	18.8	20.5	−3.6	15.4	15.9	19.1
32	5.8	26.5	9.5	25.9	26.5	28.8	3.1	26.2	24.1	28.2
33	8.5	26.1	11.3	25.4	26.2	28.8	5.7	25.4	24.0	27.4
34	8.6	26.2	11.3	25.4	26.2	28.5	5.9	25.7	24.1	27.3
35	8.0	26.6	11.1	26.3	27.5	29.7	5.6	26.3	24.9	28.5
36	8.0	29.2	11.7	28.5	29.0	31.4	5.3	28.9	26.8	30.3
37	9.9	27.5	12.6	26.8	27.6	30.2	7.1	26.8	25.6	29.6
38	−3.2	23.5	2.3	20.9	20.7	26.4	−26.4	18.7	16.9	24.9
39	−3.7	24.2	3.7	23.0	21.1	27.2	−29.8	20.7	16.7	25.3
40	−3.1	23.7	2.5	21.3	21.4	27.3	−26.9	18.7	17.2	25.3
41	−3.8	25.8	3.9	24.6	22.6	28.9	−30.8	22.2	17.9	26.9
42	−2.6	24.4	2.9	21.9	22.1	28.1	−26.8	19.0	17.9	26.3
43	−3.1	26.9	4.4	25.7	23.5	30.0	−30.5	23.1	18.8	28.3
44	−2.8	24.3	2.6	21.7	22.0	28.0	−27.1	18.8	18.0	26.3
45	3.4	28.8	7.9	30.1	29.7	38.5	−10.9	25.8	31.3	36.6
46	−15.8	−2.6	−12.4	2.9	9.9	14.4	−26.5	−4.0	8.7	12.1
47	−0.6	19.4	3.5	19.2	20.1	26.9	−11.5	15.7	21.5	25.6
48	2.9	32.4	8.2	34.1	32.4	42.5	−12.0	29.6	34.3	40.6
49	−15.5	5.1	−9.6	10.3	15.4	21.3	−25.4	4.2	14.7	18.9

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Table 18 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
50	−2.4	19.9	3.1	20.0	20.9	28.3	−14.6	16.6	22.3	26.8
51	2.9	27.9	8.1	29.0	29.7	38.2	−10.6	24.8	30.8	36.3
52	3.3	34.4	9.0	36.1	34.0	44.6	−11.3	31.8	36.1	42.5
53	−14.6	7.8	−8.3	12.6	17.6	24.0	−24.9	7.1	16.9	21.3
54	−2.5	21.0	3.5	21.0	21.9	29.5	−14.6	17.8	23.1	28.1
55	4.5	29.8	9.6	30.5	30.4	39.0	−8.2	26.2	31.9	37.4
56	−13.5	21.8	−0.6	21.9	15.6	22.1	−19.1	17.9	15.7	21.0
57	−18.0	23.3	−3.0	23.6	16.2	23.6	−23.0	19.8	16.6	22.8
58	−13.7	21.6	−0.9	21.6	15.5	22.3	−19.3	17.7	15.6	21.5
59	−14.4	24.9	−1.9	23.6	16.2	23.8	−22.0	19.9	16.4	22.9
60	−13.7	21.6	−1.1	21.5	15.6	22.5	−19.5	17.5	15.6	21.6
61	−18.2	25.7	−2.8	25.8	17.9	26.0	−23.7	22.1	18.0	25.2
62	−13.6	21.6	−1.0	21.5	15.6	22.6	−19.5	17.5	16.0	21.6
63	3.9	31.4	10.0	29.7	26.4	32.6	−20.8	29.6	24.2	32.2
64	−40.8	−0.4	−26.4	4.0	7.4	12.0	−32.5	5.2	5.6	11.1
65	−40.4	−5.2	−26.9	0.0	4.2	8.5	−31.5	1.4	2.9	7.9
66	−40.0	1.0	−26.1	5.0	8.3	13.2	−32.3	6.2	6.2	11.9
67	−38.2	−0.1	−25.7	3.9	6.2	11.0	−31.0	5.0	5.2	10.7
68	−39.7	−4.0	−26.4	1.2	5.2	9.8	−31.3	2.4	4.4	9.5
69	−40.2	1.5	−26.6	5.3	8.2	13.3	−33.0	6.3	6.7	12.9
70	−38.9	−0.3	−26.2	3.6	6.0	11.0	−31.7	4.9	5.3	10.5
71	−39.5	−3.7	−26.6	1.4	5.2	10.0	−31.6	2.4	4.2	9.3
72	−39.6	2.1	−26.2	5.8	8.7	13.9	−32.6	6.9	6.3	13.0
73	−38.3	0.1	−25.8	4.1	6.4	11.5	−31.5	5.1	5.6	11.3
74	−39.6	−3.5	−26.6	1.5	5.3	10.2	−31.7	2.5	3.6	9.1
75	−18.4	−6.5	6.3	10.1	3.5	6.8	−82.0	−24.9	−16.7	−4.4
76	−15.7	−2.4	7.9	12.2	5.5	9.2	−79.9	−21.4	−14.4	−1.3
77	−16.8	−3.5	5.6	9.8	3.6	7.2	−78.8	−21.2	−15.7	−3.0
78	−17.3	−5.2	6.9	10.7	4.3	7.6	−80.9	−23.8	−15.5	−3.4
79	−15.4	−1.4	8.1	12.7	6.0	9.8	−79.7	−20.3	−14.7	−0.6
80	−15.4	−2.1	6.9	11.1	4.8	8.4	−77.2	−19.7	−14.9	−0.9
81	−17.1	−4.6	6.9	11.1	4.5	8.0	−80.8	−23.1	−15.7	−2.8

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Table 18 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
82	−14.6	−0.6	8.8	13.4	6.7	10.6	−78.9	−19.4	−13.8	0.1
83	−15.4	−2.0	7.2	11.6	5.2	8.9	−78.0	−20.2	−14.8	−1.1
84	−16.2	−3.7	7.7	11.8	5.3	8.9	−79.9	−22.3	−15.0	−1.8
85	−11.0	5.1	−5.3	7.4	12.1	12.9	−12.4	7.3	8.7	11.3
86	−7.4	8.1	−2.2	10.1	14.5	15.3	−8.2	10.5	11.0	14.3
87	−3.7	7.8	−0.4	9.5	17.7	18.5	−5.5	8.5	14.1	16.7
88	−7.6	7.1	−2.3	9.3	14.0	14.8	−8.0	9.5	10.3	13.4
89	−10.2	6.0	−4.8	7.9	12.4	13.3	−11.9	7.8	8.9	11.9
90	−7.1	9.3	−1.8	10.8	14.6	15.5	−7.5	11.4	11.1	13.7
91	−10.3	6.0	−5.0	7.9	12.3	13.3	−12.0	7.8	8.9	11.5
92	−6.9	9.4	−1.6	11.0	14.7	15.7	−7.3	11.5	11.3	13.8
93	−6.6	9.0	−1.6	10.7	15.1	16.0	−7.7	11.0	11.5	14.5
94	−6.5	9.0	−1.5	10.7	15.3	16.1	−7.6	11.1	11.7	14.2
95	−6.8	10.1	−2.2	11.3	15.1	16.0	−8.7	11.5	11.0	14.6
96	−6.0	10.3	−0.8	12.0	15.6	16.6	−6.4	12.5	12.2	14.9
97	−6.7	10.4	−2.2	11.6	15.2	16.2	−8.8	11.9	11.2	14.3
98	−1.8	10.2	0.9	11.0	18.5	19.4	−3.8	10.5	15.0	17.8
99	−4.9	10.6	−0.4	12.0	15.8	16.8	−6.3	12.1	12.2	14.8
100	−5.5	10.3	−0.6	11.9	16.4	17.3	−6.9	12.2	12.6	15.5
101	−1.6	12.0	1.9	13.3	16.7	17.6	−3.1	13.1	12.8	16.0
102	−6.1	10.2	−0.8	11.9	15.7	16.7	−6.7	12.2	11.9	14.7
103	−5.9	11.6	−1.3	12.6	16.0	17.1	−7.6	13.1	12.1	15.4
104	−5.9	10.2	−0.7	11.9	15.9	16.7	−6.6	12.2	11.9	14.8
105	−5.2	9.5	−0.1	11.6	16.1	17.0	−6.0	11.5	12.0	15.3
106	−5.3	10.3	−0.4	12.0	16.6	17.3	−6.6	12.2	12.7	15.4
107	−17.1	5.0	−7.7	9.8	12.3	16.5	−40.3	4.2	6.3	13.9
108	−20.2	−3.4	−10.7	4.1	7.2	10.7	−42.1	−3.9	2.0	8.1
109	−16.3	7.2	−6.9	11.7	13.5	18.1	−40.0	6.0	7.8	15.4
110	−15.8	6.9	−7.3	10.3	11.6	15.9	−37.5	5.7	5.8	13.5
111	−18.4	0.0	−9.3	6.7	9.1	13.1	−41.3	−0.9	3.7	10.5
112	−15.2	9.2	−5.8	13.4	14.8	19.4	−39.4	7.6	8.4	16.5
113	−15.3	7.4	−6.8	10.8	12.1	16.4	−37.1	6.2	6.1	14.0

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Table 18 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
114	−17.8	1.5	−8.7	7.9	10.1	14.3	−41.0	0.4	4.1	11.3
115	−14.7	9.6	−5.4	13.8	15.2	19.9	−39.0	8.0	9.0	17.2
116	−15.0	7.7	−6.6	11.1	12.4	16.7	−37.1	6.2	6.5	14.1
117	−17.6	1.9	−8.6	8.2	10.3	14.6	−40.9	0.7	4.3	11.9
118	−9.2	7.9	−5.7	11.2	16.8	21.8	−21.0	6.8	15.3	19.6
119	−5.0	11.2	−2.3	11.5	14.3	19.7	−17.1	7.7	14.6	17.9
120	−11.6	3.8	−8.6	7.9	14.4	19.3	−22.8	3.1	13.0	17.0
121	−6.6	10.5	−2.9	11.2	14.3	19.5	−18.4	7.8	14.2	17.8
122	−6.2	11.5	−3.3	14.2	18.8	24.5	−19.4	10.3	17.6	21.7
123	−5.0	12.9	−2.0	13.3	15.5	21.3	−17.0	9.0	15.7	19.0
124	−8.8	8.5	−5.8	11.3	17.2	22.4	−22.5	7.6	15.5	20.1
125	−4.4	14.8	−1.0	14.6	16.7	22.2	−15.8	11.6	16.4	20.5
126	−5.6	12.2	−2.2	12.3	14.9	20.5	−17.2	9.0	14.9	18.6
127	−6.8	12.3	−3.1	15.0	19.8	25.6	−19.9	11.1	18.2	23.0
128	−28.7	4.8	−11.7	9.3	7.7	12.8	−31.5	4.8	6.2	11.4
129	−29.6	1.0	−13.0	6.2	4.7	9.5	−31.5	1.7	3.8	8.3
130	−27.5	5.9	−11.2	10.2	8.4	14.0	−30.7	5.8	7.0	12.4
131	−27.3	5.0	−12.1	9.0	7.0	12.2	−30.2	5.0	5.8	11.4
132	−28.5	2.3	−12.3	7.3	5.7	10.8	−30.8	2.8	4.9	9.7
133	−27.7	7.1	−11.2	11.1	8.9	14.7	−31.3	6.7	7.7	13.3
134	−27.3	4.9	−12.1	9.0	6.8	12.2	−30.2	5.1	5.8	11.8
135	−28.1	2.9	−12.2	7.8	5.9	11.4	−30.8	3.3	4.8	10.6
136	−27.2	7.6	−10.7	11.6	9.4	15.2	−30.9	7.2	7.7	13.9
137	−26.8	5.5	−11.8	9.4	7.2	12.8	−29.9	5.4	6.6	12.2
138	−27.8	3.6	−11.9	8.3	6.4	11.9	−30.6	3.8	5.7	11.6
139	−11.5	8.1	−3.0	12.3	14.1	18.2	−32.9	8.6	10.3	16.5
140	−9.6	12.2	−1.1	16.0	16.7	21.3	−31.8	12.1	12.7	19.0
141	−9.8	10.3	−2.2	13.3	13.8	17.8	−30.2	10.2	10.0	16.5
142	−41.3	−15.8	−31.3	−7.9	4.2	6.2	−42.7	−12.7	−4.4	1.1
143	−39.7	−16.6	−30.4	−8.5	3.3	5.3	−39.5	−12.1	−5.3	0.1
144	−38.5	−16.4	−30.0	−8.2	3.6	5.7	−38.7	−11.7	−4.5	0.4
145	−40.3	−16.4	−29.9	−8.0	4.0	6.0	−41.0	−12.8	−3.6	1.6

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Table 18 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
146	−38.8	−17.1	−29.1	−8.6	3.2	5.1	−38.1	−12.3	−4.6	0.2
147	−39.0	−17.4	−29.1	−8.3	3.4	5.5	−38.0	−12.0	−4.0	0.7
148	−16.0	−8.7	4.8	7.6	0.6	3.2	−65.6	−29.3	−17.5	−8.5
149	−20.3	−6.1	0.1	4.6	−3.8	0.0	−86.6	−33.3	−23.9	−10.2
150	−34.6	−12.9	−27.0	−6.2	4.2	7.0	−36.9	−9.1	−2.3	2.2
151	−11.6	16.9	−12.4	16.3	17.2	22.6	−20.5	15.0	13.0	20.2
152	−12.0	1.3	−5.1	8.3	5.4	9.2	−27.3	0.0	3.7	7.3
153	1.6	19.6	2.9	18.5	14.6	19.8	−17.8	11.6	13.1	17.4
154	−21.8	−7.7	−10.0	2.5	4.2	7.5	−36.6	−7.1	−0.6	3.4
155	−12.4	5.8	−5.5	10.7	10.3	14.5	−26.3	4.7	7.5	11.6
156	−5.4	13.8	1.2	15.8	13.1	17.6	−26.2	10.4	10.4	16.3
157	−8.6	11.1	−4.1	12.5	13.5	18.4	−24.3	7.5	11.2	15.8
158	−16.1	−8.7	4.7	7.5	1.1	3.8	−65.7	−29.2	−17.2	−8.3
159	−16.1	−8.6	4.6	7.5	1.0	3.7	−65.8	−29.2	−17.3	−8.3
160	−34.3	−12.6	−26.9	−6.1	4.7	7.5	−36.9	−9.1	−2.1	2.7
161	−9.6	19.5	−10.5	18.8	19.5	24.7	−16.5	19.4	15.0	22.7
162	−15.2	−3.7	−7.4	5.7	4.4	7.7	−27.1	−5.3	1.4	4.8
163	−0.3	18.7	3.0	19.4	15.3	21.0	−20.3	13.7	14.4	19.1
164	−23.8	−9.8	−13.3	0.2	3.0	5.6	−35.4	−9.0	−2.4	1.8
165	−16.6	−4.4	−8.1	5.1	4.8	8.1	−28.4	−4.4	1.3	4.6
166	−10.3	12.2	−1.4	14.5	14.6	19.6	−32.3	9.0	10.0	17.6
167	−14.6	4.8	−6.7	10.5	10.9	15.4	−29.5	2.0	8.0	12.0
168	−16.0	−8.6	4.8	7.7	1.4	4.1	−65.7	−29.1	−16.9	−7.8
169	−15.8	−8.2	5.0	7.9	1.6	4.3	−66.0	−28.9	−17.1	−8.2
170	−34.9	−13.4	−27.2	−6.7	3.2	6.2	−36.7	−9.4	−3.5	1.3
171	−31.4	−3.5	−26.9	0.6	7.9	11.8	−37.9	−2.4	1.2	7.9
172	−11.2	2.2	−1.8	12.3	7.4	11.8	−27.7	0.9	5.0	8.7
173	−6.1	14.9	−0.9	17.6	13.9	19.4	−26.5	11.8	11.9	18.1
174	−17.7	−5.8	−9.1	4.1	4.3	7.6	−29.1	−5.5	1.0	4.6
175	−17.3	7.1	−6.3	11.8	12.5	17.5	−39.1	5.4	7.6	15.2
176	−12.8	8.7	−4.0	13.2	13.5	19.0	−30.7	9.4	10.8	17.3
177	−15.5	−8.1	5.2	8.1	1.8	4.6	−65.0	−28.7	−16.7	−7.6

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Table 18 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
178	−14.5	3.4	5.4	10.7	2.7	7.2	−83.9	−18.2	−17.2	−0.7
179	−34.6	−13.1	−26.9	−6.4	3.5	6.4	−36.5	−9.2	−3.3	1.3
180	−35.1	−13.4	−27.7	−6.9	4.0	6.9	−37.8	−10.0	−3.0	2.4
181	−10.2	8.0	−2.0	15.6	10.8	16.2	−29.5	5.9	9.2	14.2
182	−9.2	9.8	−1.3	16.8	11.8	17.5	−28.9	7.7	10.3	15.7
183	−22.8	−8.9	−12.4	1.0	3.9	6.5	−34.4	−8.3	−1.3	2.8
184	−17.2	−5.4	−8.7	4.4	4.7	8.0	−28.5	−5.1	1.3	4.5
185	−17.4	4.3	−6.5	10.9	11.2	15.9	−38.5	3.3	6.2	13.2
186	−15.6	2.3	−6.2	10.1	10.1	15.0	−31.6	4.1	7.1	13.1
187	−16.6	−2.8	6.9	11.2	3.6	7.4	−79.1	−25.2	−17.1	−3.7
188	−32.7	−2.1	−27.0	1.8	10.2	14.3	−39.8	−2.7	2.9	9.3
189	−11.3	9.0	−2.4	17.2	12.0	17.3	−32.3	5.6	9.5	15.0
190	−20.4	2.9	−8.7	10.2	11.5	15.9	−43.1	0.6	5.4	12.4
191	−17.8	1.5	−8.0	10.0	10.7	15.2	−35.6	1.2	6.4	12.2
192	−15.7	0.2	8.2	13.2	5.5	9.7	−81.2	−20.9	−15.6	−0.8
193	−33.8	−2.6	−28.6	1.4	9.8	14.1	−41.6	−2.9	2.3	9.9
194	−11.3	10.2	−2.2	18.6	12.7	18.7	−33.1	6.8	10.4	15.9
195	−21.6	3.1	−8.6	10.8	11.4	16.2	−45.3	0.8	5.5	12.7
196	−19.1	1.6	−8.2	10.6	10.5	15.4	−37.9	1.9	6.5	12.3
197	−13.5	2.3	10.2	14.9	8.1	12.1	−80.7	−13.9	−12.5	2.4
198	−27.6	7.6	−25.1	7.3	13.9	18.2	−35.3	7.4	7.3	15.1
199	−5.7	17.5	−1.3	20.3	16.9	22.8	−28.1	14.5	15.1	21.4
200	−12.1	16.0	−3.5	17.8	17.8	22.9	−37.2	14.2	12.3	20.9
201	−12.9	14.6	−5.7	17.4	17.8	23.4	−29.8	13.2	15.4	21.6
202	−16.3	−4.1	5.8	9.9	2.4	5.9	−71.5	−26.9	−17.6	−5.3
203	−37.6	−9.4	−30.8	−3.8	5.9	9.4	−42.1	−7.4	−1.8	4.7
204	−15.1	1.1	−6.2	10.4	7.4	11.8	−30.8	−1.6	4.1	8.4
205	−23.1	−4.5	−10.8	5.0	6.8	10.4	−41.4	−5.4	0.6	6.0
206	−21.2	−6.1	−10.4	4.4	6.1	9.6	−35.8	−5.0	2.3	7.2
207	−17.0	−3.0	6.6	10.8	3.5	7.1	−79.3	−18.9	−16.2	−3.0
208	−27.5	3.9	−24.5	3.9	10.3	14.1	−32.2	5.4	4.0	10.6
209	−9.3	9.9	−2.9	14.9	11.4	16.3	−28.8	8.8	9.7	15.3

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Table 18 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
210	−16.8	5.8	−7.6	9.8	10.7	14.9	−38.1	5.6	5.5	12.9
211	−10.2	8.4	−4.2	11.5	11.8	16.1	−25.3	10.5	9.0	14.7
212	−17.2	−6.7	4.4	8.1	0.8	3.9	−71.4	−29.3	−18.9	−8.1
213	−36.8	−11.7	−30.1	−5.3	4.8	8.1	−40.8	−8.8	−2.5	3.1
214	−14.0	3.1	−3.2	13.5	8.9	13.7	−32.0	2.1	6.3	11.3
215	−24.9	−8.7	−11.8	2.4	5.0	8.5	−42.6	−8.6	−0.6	4.5
216	−21.3	−4.6	−10.0	6.1	5.9	9.7	−35.0	−4.8	2.1	6.3
217	−17.4	−5.2	5.8	9.9	2.0	5.4	−76.7	−26.9	−18.3	−6.5
218	−39.0	−10.6	−32.4	−4.5	5.0	8.8	−43.9	−7.9	−2.4	3.8
219	−13.6	5.7	−3.3	15.3	9.8	15.0	−32.9	4.4	7.2	12.2
220	−23.2	−3.3	−11.4	6.6	7.6	11.3	−40.8	−4.5	1.8	7.3
221	−22.9	−1.9	−11.0	8.1	8.7	13.2	−36.3	−2.0	4.8	8.8
222	−13.0	4.3	9.8	14.5	8.0	11.9	−77.5	−7.5	−12.8	2.7
223	−38.0	−9.6	−31.7	−4.0	5.8	9.7	−43.4	−7.5	−1.6	4.7
224	−9.2	12.4	−3.8	15.7	13.9	19.2	−30.0	11.2	11.6	18.0
225	−22.5	−4.8	−11.2	4.8	6.9	10.4	−38.8	−6.3	1.0	6.1
226	−20.5	−2.2	−9.8	7.6	8.9	13.3	−37.7	−1.0	4.6	10.1
227	−18.3	−7.7	4.3	7.8	−0.3	2.7	−76.3	−29.3	−19.7	−9.3
228	−33.6	−12.5	−27.5	−6.5	3.4	6.2	−36.2	−8.9	−2.3	2.1
229	−17.0	−1.2	−7.7	8.0	5.1	8.7	−32.3	−2.7	1.9	5.2
230	−23.0	−8.1	−13.9	0.0	2.6	5.0	−34.0	−8.7	−2.7	1.9
231	−20.6	−9.1	−7.8	2.7	2.6	6.0	−31.9	−5.6	−0.3	3.1
232	−17.1	−6.2	5.5	9.0	1.3	4.3	−75.9	−27.3	−18.4	−7.5
233	−36.2	−8.9	−29.5	−3.3	6.1	9.7	−40.6	−6.1	−0.7	5.2
234	−12.5	5.9	−2.3	15.6	9.8	14.6	−31.8	5.0	7.4	12.1
235	−25.3	−6.3	−14.4	3.1	6.4	9.6	−42.1	−6.8	0.9	6.2
236	−19.6	−4.4	−9.8	5.5	4.4	8.2	−32.0	−5.3	1.2	4.3
MAXD	−41.3	34.4	−32.4	36.1	34.0	44.6	−86.6	−33.3	36.1	42.5
MD	−15.5	6.1	−5.0	11.4	11.5	15.6	−33.7	2.7	5.5	12.0
MAD	16.5	10.5	9.6	12.4	11.5	15.6	34.3	12.5	11.5	13.3

Table 19: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the TPSS0 functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−14.7	22.9	−5.0	22.1	18.2	25.0	−10.9	22.6	19.9	24.9
2	−18.7	23.5	−7.4	22.9	18.7	26.2	−13.6	24.1	20.4	26.2
3	−16.4	21.2	−6.6	20.6	17.4	24.3	−12.4	21.3	19.1	24.4
4	−19.1	24.5	−7.5	23.9	19.6	27.3	−14.1	25.2	21.2	27.2
5	−17.3	23.4	−7.0	22.5	19.0	26.4	−13.2	23.4	20.6	26.2
6	−19.1	25.0	−7.5	24.4	20.0	27.9	−14.2	25.6	21.5	27.7
7	−17.0	23.7	−6.7	22.8	19.5	26.7	−13.0	23.6	20.6	26.5
8	−3.1	11.6	15.3	19.7	9.8	14.6	−65.3	−6.7	−6.0	7.3
9	−2.6	13.0	16.4	21.0	11.2	16.2	−66.7	−3.7	−4.9	9.2
10	−12.8	−2.4	10.2	13.7	5.4	9.1	−67.6	−18.8	−11.0	−0.3
11	−10.9	0.0	11.2	14.7	6.7	10.5	−67.0	−15.4	−9.7	1.5
12	−2.7	12.1	15.7	20.1	10.5	15.4	−65.4	−6.3	−5.3	8.2
13	−1.1	14.7	17.9	22.7	12.9	18.0	−65.4	−2.2	−3.3	11.2
14	−12.4	−2.0	10.5	14.0	5.6	9.5	−67.4	−18.5	−10.8	0.1
15	−9.3	3.3	13.0	16.9	8.8	12.9	−67.7	−10.5	−7.7	4.2
16	−0.5	15.7	17.8	22.5	13.1	18.2	−64.8	−2.2	−3.1	11.5
17	−0.7	15.2	18.3	23.2	13.4	18.5	−65.2	−1.8	−2.9	11.9
18	−11.9	−1.0	11.0	14.9	6.3	10.3	−67.2	−17.5	−10.2	1.2
19	−8.7	4.5	13.5	17.7	9.3	13.6	−67.7	−9.0	−7.7	5.1
20	−0.1	16.1	18.1	22.9	13.5	18.7	−64.9	−1.9	−3.1	11.8
21	13.5	29.5	16.7	29.6	29.9	32.5	11.8	30.0	29.5	31.9
22	−1.9	9.5	3.8	14.6	17.2	18.8	−1.0	13.6	16.5	18.2
23	14.1	30.8	17.3	31.1	31.7	34.1	12.6	31.2	30.9	33.6
24	12.1	28.7	15.5	29.2	29.3	31.5	10.4	29.2	28.5	31.2
25	12.6	29.9	16.1	30.1	30.4	32.9	10.6	30.2	29.5	32.1
26	12.3	28.2	15.7	28.6	28.9	31.3	10.7	28.5	28.3	30.5
27	13.4	29.4	16.5	29.3	30.0	32.5	11.4	29.5	29.3	31.9
28	15.0	31.1	18.1	31.0	31.2	33.8	13.3	31.4	30.8	33.2
29	14.5	31.4	17.7	31.6	32.1	34.7	13.0	31.7	30.8	33.6

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Table 19 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
30	14.0	32.6	17.8	32.5	32.5	35.1	12.6	32.8	31.7	34.4
31	4.7	19.1	9.9	22.4	24.9	26.8	5.3	22.5	23.4	25.9
32	13.9	32.8	17.7	32.9	33.0	35.6	12.2	33.2	32.0	35.1
33	15.4	31.7	18.4	31.5	31.7	34.6	13.4	31.5	31.1	33.9
34	15.6	31.8	18.6	31.6	31.9	34.4	13.7	31.8	31.2	33.8
35	15.9	32.9	19.0	33.2	33.7	36.3	14.1	33.1	32.6	35.6
36	16.3	35.6	20.0	35.6	35.6	38.2	14.5	36.0	34.5	37.4
37	16.8	33.0	19.7	32.9	33.1	36.0	14.8	32.8	32.7	35.7
38	3.0	27.8	8.3	25.5	25.0	31.2	−18.5	23.6	23.2	29.9
39	3.0	28.9	10.0	28.0	25.7	32.3	−21.2	26.1	23.9	31.3
40	2.9	27.9	8.4	25.9	25.6	32.0	−19.1	23.6	24.0	30.7
41	3.1	30.6	10.5	29.8	27.4	34.2	−21.8	27.7	25.4	33.2
42	3.5	28.6	8.9	26.5	26.3	32.8	−19.0	23.9	24.5	31.6
43	3.7	31.7	11.0	30.8	28.2	35.2	−21.5	28.6	26.4	34.5
44	3.3	28.5	8.6	26.3	26.2	32.8	−19.3	23.7	24.4	31.4
45	11.7	35.4	16.4	37.5	36.0	45.6	−0.7	33.2	39.2	44.2
46	−8.8	3.6	−5.4	9.3	14.9	19.8	−17.8	2.7	14.9	17.9
47	6.9	25.3	11.0	25.7	25.5	33.1	−2.2	22.5	28.4	32.3
48	12.5	40.0	18.0	42.5	39.6	50.7	−0.3	38.1	43.5	49.1
49	−7.1	12.1	−1.2	17.7	21.2	27.8	−15.2	11.8	20.4	24.0
50	5.8	26.2	11.1	26.9	26.6	34.9	−4.5	23.8	29.9	33.9
51	11.7	34.9	17.1	36.9	36.5	45.9	0.2	32.8	39.6	44.5
52	13.2	42.2	19.1	44.7	41.3	53.1	0.7	40.6	45.4	51.5
53	−5.5	15.3	0.6	20.5	23.9	31.0	−14.0	15.3	24.7	29.0
54	5.9	27.4	11.8	28.1	27.8	36.3	−4.3	25.1	30.6	35.2
55	13.2	36.6	18.5	38.3	37.1	46.5	2.3	33.9	40.1	44.9
56	−6.3	26.5	6.2	26.8	19.4	26.8	−11.0	23.1	21.7	26.9
57	−9.5	28.8	4.8	29.3	20.7	29.2	−13.6	25.8	23.6	28.8
58	−6.6	26.3	5.9	26.5	19.2	27.0	−11.2	22.8	21.8	26.7
59	−6.1	30.5	6.1	29.5	20.9	29.6	−12.6	25.9	23.5	29.7
60	−6.5	26.4	5.7	26.5	19.4	27.2	−11.4	22.7	22.0	27.0
61	−9.3	31.5	5.5	31.8	22.6	31.9	−13.8	28.4	25.2	31.5

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Table 19 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
62	−6.5	26.4	5.8	26.5	19.4	27.3	−11.4	22.6	22.0	27.0
63	10.1	35.7	15.9	34.4	30.8	37.6	−12.7	34.6	30.4	38.1
64	−32.1	5.5	−18.2	9.8	12.1	17.4	−23.8	11.1	12.0	16.7
65	−32.1	0.6	−19.1	5.7	8.7	13.6	−23.3	7.1	9.0	13.3
66	−31.4	6.8	−17.8	10.9	13.0	18.5	−23.7	12.0	13.1	18.2
67	−29.9	5.6	−17.6	9.8	11.0	16.4	−22.5	10.8	11.3	16.3
68	−31.5	1.7	−18.5	7.0	9.8	15.0	−23.1	8.1	10.3	15.0
69	−31.5	7.3	−18.3	11.1	12.9	18.7	−24.3	12.2	13.3	18.7
70	−30.5	5.4	−18.0	9.6	10.8	16.4	−23.2	10.7	11.5	16.5
71	−31.3	2.0	−18.7	7.2	9.8	15.2	−23.3	8.1	10.3	15.0
72	−30.9	7.9	−17.8	11.7	13.5	19.3	−23.8	12.8	13.5	19.4
73	−30.0	5.9	−17.7	10.0	11.1	16.9	−23.0	10.9	11.9	17.1
74	−31.3	2.2	−18.6	7.4	10.0	15.5	−23.4	8.2	10.5	15.3
75	−11.9	−1.3	12.2	15.5	7.2	10.9	−71.7	−18.4	−9.3	1.4
76	−9.5	2.4	13.5	17.4	9.1	13.2	−69.9	−15.3	−7.3	4.8
77	−10.1	1.8	11.6	15.4	7.7	11.7	−68.3	−14.7	−8.1	3.1
78	−11.1	−0.3	12.6	16.0	7.9	11.6	−70.8	−17.6	−8.5	2.1
79	−9.1	3.4	13.8	18.0	9.6	13.9	−69.6	−14.2	−7.1	5.8
80	−8.8	3.1	12.8	16.6	8.9	12.9	−66.8	−13.2	−7.3	4.7
81	−10.8	0.4	12.6	16.3	8.1	12.0	−70.6	−16.9	−8.4	3.2
82	−8.3	4.3	14.5	18.7	10.4	14.7	−68.8	−13.4	−6.6	5.9
83	−8.7	3.3	13.1	17.2	9.3	13.4	−67.6	−13.7	−7.2	5.0
84	−9.9	1.3	13.4	17.2	9.0	12.9	−69.7	−16.0	−7.8	4.4
85	−3.6	10.9	1.9	13.5	17.4	18.4	−4.2	13.6	14.8	17.2
86	0.4	14.3	5.3	16.4	20.2	21.1	0.4	17.1	17.4	19.9
87	2.3	12.8	5.6	14.9	22.3	23.3	1.1	13.9	19.8	21.8
88	−0.3	13.0	5.0	15.5	19.5	20.4	0.2	15.9	16.5	18.6
89	−3.0	11.6	2.3	13.9	17.7	18.7	−3.8	13.9	14.6	17.6
90	0.7	15.5	5.9	17.4	20.5	21.6	1.1	18.1	17.8	20.2
91	−3.2	11.6	2.2	13.9	17.6	18.7	−3.9	13.9	14.8	17.6
92	0.9	15.6	6.0	17.6	20.6	21.7	1.3	18.2	18.0	20.4
93	0.8	14.9	5.7	16.9	20.7	21.6	0.7	17.5	17.8	20.7

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Table 19 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
94	1.0	14.9	5.8	17.0	20.8	21.7	0.8	17.6	17.9	20.4
95	0.7	16.0	5.4	17.7	20.8	21.9	−0.3	17.9	17.5	20.9
96	1.7	16.5	6.9	18.5	21.5	22.6	2.1	19.2	18.7	21.7
97	0.8	16.3	5.4	18.0	21.0	22.1	−0.3	18.3	17.8	20.2
98	3.9	14.9	6.8	16.2	23.0	24.0	2.7	15.8	20.6	23.2
99	2.3	16.3	6.8	18.1	21.2	22.3	1.7	18.3	18.4	20.8
100	2.0	16.2	6.7	18.1	22.0	22.9	1.6	18.7	18.9	21.7
101	4.6	17.0	8.1	18.6	21.4	22.5	3.8	18.5	18.3	21.3
102	1.7	16.4	6.9	18.5	21.6	22.7	1.8	18.9	18.6	21.3
103	1.7	17.6	6.4	19.1	21.9	23.1	0.9	19.6	18.7	21.6
104	1.8	16.4	7.0	18.5	21.8	22.7	2.0	18.9	18.6	21.4
105	1.8	15.1	6.8	17.6	21.5	22.4	1.8	17.6	18.1	21.3
106	2.2	16.2	6.9	18.2	22.2	23.0	1.8	18.7	19.0	21.6
107	−9.9	10.6	−0.9	15.3	17.2	21.8	−31.2	10.3	13.5	20.1
108	−13.3	2.2	−4.2	9.5	11.9	15.8	−33.6	2.1	8.7	13.9
109	−9.2	12.6	−0.3	17.1	18.3	23.3	−31.0	11.9	14.9	21.3
110	−8.7	12.4	−0.6	15.8	16.4	21.1	−28.7	11.6	12.6	19.3
111	−11.7	5.3	−3.0	12.0	13.6	18.0	−32.8	4.8	10.4	16.2
112	−8.2	14.4	0.8	18.8	19.5	24.6	−30.4	13.4	15.5	22.3
113	−8.3	12.7	−0.2	16.2	16.8	21.5	−28.4	11.9	13.0	19.8
114	−11.0	6.8	−2.3	13.2	14.7	19.3	−32.5	6.2	10.9	17.0
115	−7.7	14.8	1.2	19.1	19.9	25.0	−30.1	13.8	16.0	23.0
116	−8.0	13.0	0.0	16.5	17.1	21.9	−28.5	11.9	13.1	19.5
117	−10.8	7.2	−2.1	13.5	14.9	19.7	−32.4	6.4	11.2	17.7
118	−1.9	14.0	1.7	17.7	22.1	27.6	−11.9	13.5	21.7	25.5
119	1.5	16.2	4.1	16.8	18.6	24.6	−8.9	13.4	20.2	22.4
120	−4.3	10.1	−1.0	14.6	19.8	25.3	−13.7	9.9	19.6	23.4
121	0.4	15.8	3.9	16.8	19.0	24.8	−9.7	13.9	20.2	23.6
122	1.0	17.4	4.1	20.6	24.0	30.3	−10.4	16.9	24.5	28.8
123	1.6	17.8	4.5	18.7	19.9	26.3	−8.8	14.7	21.4	24.3
124	−0.9	15.1	2.2	18.4	23.0	28.7	−12.7	14.9	22.5	26.9
125	3.2	20.6	6.6	20.9	22.0	28.2	−6.5	18.2	22.7	26.7

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Table 19 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
126	1.5	17.5	4.8	18.1	19.8	26.0	−8.3	15.2	20.9	24.3
127	1.1	18.8	4.9	21.9	25.6	32.0	−10.1	18.3	25.1	29.8
128	−20.4	10.4	−4.1	14.9	12.1	17.9	−22.3	10.8	12.7	17.5
129	−21.5	6.5	−5.6	11.7	9.0	14.3	−22.7	7.5	9.9	13.7
130	−19.3	11.4	−3.6	15.8	12.9	19.2	−21.6	11.7	13.5	18.0
131	−19.2	10.5	−4.4	14.7	11.5	17.4	−21.3	10.9	12.2	17.0
132	−20.6	7.7	−4.9	12.7	9.9	15.7	−22.0	8.5	10.7	15.0
133	−19.4	12.7	−3.5	16.7	13.3	19.9	−22.1	12.6	14.1	18.8
134	−19.3	10.4	−4.5	14.6	11.2	17.4	−21.3	10.8	12.1	17.2
135	−20.1	8.4	−4.8	13.3	10.2	16.3	−22.0	9.0	10.9	16.4
136	−18.9	13.2	−2.9	17.3	13.8	20.5	−21.6	13.1	14.6	19.9
137	−18.8	11.0	−4.1	15.1	11.6	17.9	−21.1	11.2	12.7	18.3
138	−19.8	9.0	−4.5	13.8	10.6	16.9	−21.8	9.6	11.7	17.2
139	−4.9	13.3	3.2	17.6	18.9	23.3	−24.4	14.2	16.6	22.3
140	−3.1	17.1	5.0	21.1	21.3	26.4	−23.4	17.5	18.9	24.6
141	−3.4	15.2	3.8	18.4	18.4	22.8	−22.2	15.6	16.0	22.0
142	−33.7	−10.0	−23.9	−2.1	8.7	10.9	−34.8	−6.9	1.7	6.4
143	−32.8	−11.3	−23.6	−3.2	7.5	9.7	−32.5	−6.8	0.3	6.0
144	−31.8	−11.2	−23.4	−3.0	7.5	9.8	−31.8	−6.6	0.7	5.3
145	−32.2	−10.1	−22.0	−1.7	8.9	11.1	−32.6	−6.4	1.8	7.0
146	−31.3	−11.2	−21.7	−2.7	7.8	9.9	−30.5	−6.4	0.5	6.0
147	−31.6	−11.5	−21.9	−2.6	7.8	10.0	−30.5	−6.2	0.8	5.9
148	−9.0	−2.4	10.6	13.2	5.0	7.9	−55.8	−22.0	−10.1	−2.2
149	−13.2	−0.4	6.3	10.3	0.8	5.0	−75.8	−26.1	−15.6	−3.7
150	−27.6	−7.7	−20.2	−1.1	7.6	10.7	−29.2	−3.9	2.5	6.9
151	−4.9	21.7	−5.2	21.4	21.1	27.1	−12.9	20.1	19.3	25.6
152	−6.6	5.6	−0.1	12.6	8.5	12.7	−20.2	4.9	8.4	11.5
153	7.0	23.7	8.3	23.1	18.4	24.1	−10.8	16.4	18.6	22.2
154	−16.0	−3.0	−4.8	6.9	7.8	11.3	−29.8	−2.3	4.2	8.1
155	−6.2	10.7	0.7	15.8	14.2	18.9	−18.4	10.1	12.8	17.2
156	−0.5	17.5	5.8	19.5	16.2	21.2	−19.9	14.4	14.8	20.1
157	−2.1	16.1	2.5	17.8	17.8	23.3	−16.1	13.2	17.0	21.3

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Table 19 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
158	−9.1	−2.4	10.5	13.1	5.4	8.4	−55.9	−22.0	−9.7	−2.0
159	−9.1	−2.4	10.4	13.0	5.4	8.3	−56.0	−22.0	−9.7	−2.0
160	−27.4	−7.5	−20.0	−1.0	8.0	11.2	−29.2	−3.9	2.5	6.9
161	−2.8	24.4	−3.1	24.1	23.5	29.2	−8.8	24.6	21.7	28.4
162	−9.5	1.0	−2.0	10.3	7.8	11.5	−20.1	−0.1	6.2	8.8
163	5.1	22.7	8.3	23.7	18.8	25.0	−13.1	18.4	19.7	24.6
164	−18.1	−5.1	−8.2	4.5	6.6	9.4	−28.6	−4.1	2.5	6.1
165	−10.3	0.9	−2.0	10.3	9.0	12.6	−20.7	1.3	6.7	9.7
166	−4.3	16.5	4.1	18.9	18.3	23.7	−25.0	13.7	16.1	22.6
167	−7.7	10.1	−0.1	16.0	15.1	20.1	−21.1	7.9	14.2	18.6
168	−9.1	−2.3	10.5	13.2	5.7	8.7	−56.0	−21.9	−9.6	−1.6
169	−8.9	−2.0	10.7	13.4	5.9	8.8	−56.3	−21.7	−9.6	−1.5
170	−27.9	−8.1	−20.3	−1.6	6.7	10.0	−29.1	−4.1	1.3	5.9
171	−23.6	2.1	−19.0	6.3	11.8	16.3	−29.2	3.4	6.7	13.1
172	−5.2	7.2	3.8	17.1	11.0	15.8	−20.1	6.3	10.6	14.5
173	0.6	19.9	5.6	23.0	18.3	24.3	−17.8	17.5	17.8	23.6
174	−11.4	−0.5	−3.2	9.2	8.4	12.0	−21.6	0.2	6.2	9.1
175	−9.8	12.8	0.5	17.4	17.3	22.8	−30.1	11.4	14.1	21.1
176	−4.6	15.2	3.9	19.8	18.9	24.9	−20.9	16.3	18.0	23.9
177	−8.6	−1.9	10.9	13.6	6.1	9.1	−55.3	−21.5	−9.1	−1.2
178	−7.6	8.5	11.5	16.3	7.1	12.0	−73.0	−11.7	−9.1	5.4
179	−27.7	−7.9	−20.1	−1.3	7.0	10.2	−28.8	−3.9	1.5	6.0
180	−28.2	−8.3	−20.9	−1.9	7.3	10.5	−30.2	−4.8	1.7	6.5
181	−3.1	13.6	4.8	21.3	15.2	21.2	−20.5	12.1	15.2	20.3
182	−2.0	15.5	5.6	22.5	16.3	22.5	−19.8	14.0	16.6	21.6
183	−17.2	−4.3	−7.4	5.3	7.4	10.3	−27.7	−3.6	3.4	7.1
184	−11.0	−0.2	−2.8	9.5	8.7	12.3	−21.1	0.5	6.5	9.8
185	−10.4	9.7	−0.1	16.1	15.7	20.9	−30.0	9.0	12.4	18.8
186	−7.9	8.7	1.2	16.3	15.2	20.4	−22.4	10.6	10.1	15.5
187	−7.5	4.9	14.7	18.6	9.6	13.8	−66.6	−16.3	−7.4	4.3
188	−24.0	4.2	−18.4	8.2	14.9	19.5	−30.3	3.9	9.7	16.1
189	−3.2	15.6	5.3	23.7	17.3	23.1	−22.1	13.0	16.9	21.7

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Table 19 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
190	−12.0	9.7	−1.0	16.8	17.3	22.0	−33.1	7.9	12.9	19.4
191	−9.0	8.9	0.3	17.2	16.7	21.5	−25.3	9.0	14.5	20.0
192	−6.4	8.0	16.3	20.8	11.8	16.4	−68.2	−11.9	−5.6	7.5
193	−24.8	4.0	−19.5	8.2	14.9	19.7	−31.6	4.0	9.1	16.3
194	−2.6	17.3	6.0	25.6	18.5	25.0	−22.3	14.6	17.9	23.2
195	−13.0	10.0	−0.8	17.3	17.3	22.5	−35.1	8.0	13.0	19.2
196	−9.8	9.3	0.6	18.1	16.8	22.2	−27.0	9.9	14.9	20.3
197	−7.3	6.8	15.6	19.9	11.6	16.0	−70.5	−8.1	−5.3	7.8
198	−20.6	11.9	−17.7	12.2	17.5	22.3	−26.9	12.4	13.3	20.8
199	1.6	22.9	5.9	26.0	21.8	28.2	−18.3	20.8	22.7	28.3
200	−4.9	21.2	3.2	23.0	22.6	28.2	−28.0	20.0	19.5	26.4
201	−4.6	20.7	2.5	23.9	23.3	29.4	−19.6	20.1	22.3	27.9
202	−7.4	3.7	13.8	17.5	8.7	12.6	−59.4	−17.9	−7.6	3.1
203	−29.0	−3.0	−22.0	2.7	10.6	14.6	−32.7	−0.7	4.8	10.7
204	−7.9	7.1	0.8	16.4	12.2	17.0	−21.9	5.0	10.3	14.3
205	−15.7	1.6	−3.9	10.9	11.9	15.8	−32.6	1.0	7.3	12.1
206	−12.8	1.1	−2.4	11.5	11.8	15.7	−26.2	2.5	8.7	13.3
207	−10.2	2.2	12.7	16.4	7.6	11.6	−68.7	−12.3	−8.4	3.1
208	−20.9	8.1	−17.4	8.7	13.7	18.0	−24.2	10.3	9.3	15.7
209	−2.2	15.4	4.0	20.6	16.2	21.6	−19.4	15.1	16.5	21.4
210	−10.1	10.9	−1.2	15.0	15.2	19.8	−29.6	11.2	12.3	18.7
211	−3.7	13.5	2.2	16.9	16.3	20.9	−17.1	16.1	15.0	20.1
212	−8.8	0.7	11.9	15.2	6.8	10.0	−60.0	−20.8	−9.5	−0.2
213	−29.1	−5.9	−22.3	0.5	8.8	12.5	−32.3	−2.9	3.3	8.9
214	−6.7	9.1	3.8	19.4	13.5	18.7	−22.8	8.7	12.7	17.2
215	−18.4	−3.4	−6.0	7.4	9.0	12.8	−34.9	−3.1	5.1	9.8
216	−13.8	1.6	−2.8	12.2	10.6	14.8	−26.2	1.8	8.4	11.8
217	−8.8	2.2	13.3	17.1	7.9	11.6	−64.8	−18.4	−8.8	1.6
218	−30.9	−4.6	−24.1	1.6	9.3	13.5	−34.9	−1.7	3.5	9.9
219	−6.1	11.7	3.9	21.3	14.7	20.2	−23.3	11.1	13.8	18.6
220	−15.9	2.6	−4.7	12.3	12.4	16.4	−32.0	1.8	8.3	13.2
221	−14.4	5.0	−2.8	15.0	14.2	19.2	−26.3	5.4	12.4	16.5

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Table 19 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
222	−6.6	8.9	15.6	19.9	11.9	16.2	−67.0	−1.7	−5.2	8.4
223	−30.0	−3.8	−23.5	2.1	10.0	14.2	−34.5	−1.5	4.2	10.3
224	−1.6	18.2	3.9	22.0	19.2	25.0	−20.0	17.9	19.8	24.7
225	−16.3	0.3	−5.5	9.6	11.0	14.8	−31.4	−1.0	6.6	11.2
226	−12.5	4.4	−2.0	14.3	14.2	19.0	−28.1	6.1	11.5	16.5
227	−10.0	−0.5	11.4	14.5	5.2	8.5	−64.8	−21.0	−10.6	−1.6
228	−27.1	−7.6	−21.0	−1.6	6.4	9.5	−29.2	−4.1	2.0	6.1
229	−10.4	4.1	−1.5	13.3	9.2	13.1	−24.2	3.1	7.4	11.3
230	−17.4	−3.6	−8.8	4.2	6.3	8.9	−27.8	−4.1	2.3	6.3
231	−13.9	−3.2	−1.8	8.0	6.7	10.4	−24.4	0.2	5.2	8.4
232	−9.1	0.7	12.3	15.5	6.5	9.8	−64.7	−19.5	−9.7	−0.1
233	−28.4	−3.3	−21.8	2.4	9.9	13.9	−32.1	−0.4	4.9	10.6
234	−5.4	11.6	4.5	21.3	14.3	19.5	−22.6	11.4	13.6	18.8
235	−18.8	−1.3	−8.4	8.0	10.3	13.8	−34.4	−1.4	6.6	11.1
236	−12.6	1.5	−3.1	11.2	8.9	13.0	−24.0	0.9	7.1	10.0
MAXD	−33.7	42.2	−24.1	44.7	41.3	53.1	−75.8	40.6	45.4	51.5
MD	−8.1	11.7	2.0	17.2	16.3	20.8	−24.8	8.9	12.2	18.0
MAD	11.4	13.2	9.4	17.4	16.3	20.8	26.7	14.6	14.9	18.1

Table 20: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the TPSSh functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−17.8	23.8	−6.6	23.4	20.3	27.1	−13.6	23.7	20.5	26.8
2	−22.1	24.6	−9.0	24.5	20.9	28.5	−16.4	25.6	21.1	28.1
3	−19.5	22.1	−8.2	21.9	19.5	26.4	−15.1	22.5	19.7	25.9
4	−22.5	25.7	−9.2	25.6	22.0	29.7	−16.9	26.7	22.0	29.2
5	−20.7	24.4	−8.7	24.0	21.2	28.6	−16.1	24.7	21.3	28.1
6	−22.4	26.4	−9.2	26.1	22.4	30.3	−17.1	27.2	22.4	29.7
7	−20.3	24.8	−8.4	24.2	21.7	28.9	−15.9	24.9	21.5	28.4

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Table 20 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
8	−7.4	9.2	13.0	18.0	8.5	13.6	−72.7	−9.5	−9.7	5.4
9	−6.6	11.0	14.3	19.6	10.2	15.5	−73.9	−6.0	−8.3	7.7
10	−15.1	−3.4	9.6	13.5	5.9	9.9	−72.4	−19.7	−12.7	−0.6
11	−13.3	−0.9	10.4	14.5	7.2	11.3	−72.0	−16.3	−11.4	1.0
12	−6.9	9.9	13.5	18.5	9.3	14.5	−72.7	−8.9	−8.7	6.5
13	−5.0	12.9	15.9	21.4	11.8	17.4	−72.6	−4.4	−6.6	9.7
14	−14.7	−2.9	9.9	13.9	6.1	10.3	−72.2	−19.4	−12.2	−0.2
15	−11.6	2.8	12.4	16.9	9.3	13.8	−72.7	−11.0	−9.3	4.5
16	−4.4	13.9	15.8	21.2	12.1	17.6	−71.9	−4.4	−6.4	10.0
17	−4.5	13.5	16.4	22.0	12.4	17.9	−72.3	−3.9	−6.1	10.3
18	−14.1	−1.8	10.5	14.9	6.9	11.2	−71.8	−18.3	−11.6	1.0
19	−10.9	4.1	13.0	17.8	9.9	14.6	−72.6	−9.3	−9.0	5.4
20	−4.0	14.4	16.2	21.7	12.5	18.1	−71.9	−4.1	−6.0	10.5
21	12.2	29.7	16.1	29.9	31.0	33.5	10.0	30.0	29.6	32.4
22	−3.8	8.6	2.7	14.2	17.8	19.4	−3.1	12.8	15.9	18.1
23	13.4	31.5	17.2	31.9	33.3	35.8	11.3	31.6	31.1	34.7
24	11.1	29.1	15.2	29.8	30.8	32.9	8.9	29.4	28.7	31.9
25	11.3	30.2	15.5	30.6	31.7	34.1	8.8	30.3	29.5	33.1
26	11.2	28.5	15.1	29.0	30.2	32.5	9.0	28.5	28.1	31.3
27	12.1	29.6	15.8	29.6	31.1	33.6	9.5	29.5	29.3	32.4
28	13.9	31.5	17.6	31.5	32.5	35.1	11.8	31.6	31.0	34.2
29	13.8	32.1	17.6	32.5	33.9	36.4	11.7	32.1	31.7	35.2
30	13.1	33.3	17.6	33.3	34.1	36.7	11.1	33.2	32.1	35.9
31	3.4	19.0	9.3	22.7	26.1	28.0	3.5	22.5	23.7	26.6
32	12.9	33.6	17.4	33.7	34.6	37.1	10.7	33.7	32.4	36.3
33	14.6	32.3	18.1	32.3	33.3	36.1	12.2	31.9	31.5	35.1
34	14.7	32.3	18.3	32.2	33.3	35.8	12.3	32.1	31.6	34.9
35	15.2	33.7	19.0	34.1	35.5	38.0	13.0	33.6	33.2	36.8
36	15.4	36.5	19.8	36.5	37.3	39.9	13.1	36.6	35.2	39.1
37	16.1	33.7	19.6	33.7	34.7	37.6	13.6	33.3	33.4	37.0
38	3.3	30.6	10.0	28.6	28.3	34.4	−19.6	26.3	24.8	32.6
39	3.0	31.6	11.6	30.9	28.9	35.5	−22.8	28.6	25.4	33.9

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Table 20 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
40	3.3	30.8	10.2	29.1	29.0	35.4	−20.3	26.3	25.5	33.4
41	3.2	33.5	12.2	33.0	30.8	37.5	−23.4	30.5	27.0	36.0
42	3.9	31.6	10.8	29.8	29.8	36.2	−20.1	26.6	26.3	34.3
43	3.8	34.7	12.8	34.1	31.7	38.6	−23.1	31.5	28.0	37.1
44	3.8	31.5	10.6	29.7	29.7	36.2	−20.2	26.5	26.4	34.4
45	11.3	37.3	17.4	39.6	38.7	48.1	−2.7	34.7	40.7	45.9
46	−9.6	3.6	−5.1	10.0	16.3	21.1	−19.8	2.8	15.4	18.6
47	6.6	27.3	12.4	28.3	28.6	36.0	−3.6	24.4	29.5	33.9
48	11.9	42.2	19.0	45.0	42.6	53.5	−2.5	39.9	45.2	51.1
49	−8.2	12.7	−1.0	18.8	23.1	29.5	−17.6	12.2	23.1	27.2
50	5.3	28.4	12.6	29.7	29.9	38.0	−6.0	25.9	31.2	35.7
51	11.5	37.2	18.5	39.4	39.5	48.7	−1.4	34.7	41.5	46.5
52	12.7	44.6	20.2	47.4	44.5	56.1	−1.4	42.5	47.3	53.5
53	−6.6	16.2	1.1	22.0	26.0	33.0	−16.4	16.0	25.7	30.3
54	5.5	29.8	13.3	31.0	31.1	39.5	−5.8	27.4	32.4	37.2
55	12.9	39.0	19.8	40.8	40.1	49.3	0.7	35.8	42.1	47.0
56	−8.8	27.8	5.5	28.4	21.4	28.9	−15.0	23.9	22.1	28.6
57	−12.3	30.4	4.1	31.3	23.1	31.6	−18.0	27.0	23.9	31.0
58	−9.0	27.6	5.2	28.2	21.3	29.2	−15.1	23.7	22.4	28.7
59	−8.9	31.8	5.3	31.3	23.0	31.7	−17.1	26.9	24.1	31.1
60	−8.8	27.8	5.2	28.2	21.5	29.4	−15.3	23.6	22.6	29.0
61	−12.1	33.3	4.8	34.0	25.2	34.4	−18.3	29.8	26.1	33.9
62	−8.7	27.8	5.3	28.4	21.6	29.6	−15.2	23.6	22.7	29.2
63	12.1	40.1	19.2	38.7	35.1	41.7	−12.2	38.9	33.5	41.8
64	−37.2	4.7	−21.4	9.7	13.1	18.4	−28.2	10.9	11.5	17.3
65	−36.9	−0.5	−22.2	5.3	9.5	14.4	−27.5	6.6	8.2	13.4
66	−36.5	6.1	−21.0	10.8	14.0	19.6	−28.1	11.9	12.3	18.5
67	−34.8	4.8	−20.8	9.6	11.9	17.3	−26.9	10.6	10.6	16.3
68	−36.4	0.7	−21.7	6.6	10.6	15.8	−27.3	7.6	9.5	14.7
69	−36.6	6.7	−21.6	11.2	14.0	19.8	−28.7	12.2	12.5	18.8
70	−35.5	4.6	−21.2	9.5	11.7	17.4	−27.6	10.4	11.2	16.8
71	−36.1	1.1	−21.8	6.9	10.6	16.1	−27.5	7.7	9.8	15.3

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Table 20 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
72	−35.9	7.4	−21.0	11.8	14.7	20.5	−28.2	12.7	13.0	19.5
73	−34.9	5.1	−20.8	9.9	12.1	17.8	−27.3	10.6	11.2	16.9
74	−36.0	1.3	−21.7	7.2	10.8	16.4	−27.5	7.9	9.7	15.3
75	−15.5	−3.4	9.9	13.8	6.3	10.2	−78.2	−20.7	−12.5	−0.5
76	−13.0	0.6	11.4	15.9	8.3	12.8	−76.3	−17.4	−10.6	2.5
77	−13.6	−0.1	9.5	13.9	6.8	11.1	−74.7	−16.8	−11.4	1.2
78	−14.6	−2.3	10.4	14.4	7.1	11.1	−77.2	−19.7	−11.5	0.3
79	−12.5	1.8	11.8	16.6	8.9	13.5	−76.0	−16.2	−10.0	3.7
80	−12.3	1.4	10.8	15.1	8.1	12.4	−73.2	−15.2	−10.2	2.7
81	−14.3	−1.5	10.5	14.9	7.3	11.6	−76.9	−18.9	−11.2	1.1
82	−11.7	2.7	12.6	17.4	9.7	14.4	−75.2	−15.2	−9.1	4.6
83	−12.2	1.5	11.1	15.8	8.5	12.9	−74.0	−15.7	−9.9	3.3
84	−13.3	−0.5	11.4	15.7	8.2	12.5	−76.0	−18.0	−10.3	2.2
85	−6.3	9.8	0.0	12.6	17.4	18.3	−7.4	12.4	13.8	16.7
86	−2.1	13.3	3.5	15.7	20.5	21.4	−2.7	16.0	16.8	19.7
87	1.8	13.4	5.6	15.6	23.4	24.3	0.4	14.6	19.9	22.4
88	−2.4	12.2	3.5	14.9	20.1	20.9	−2.5	14.9	16.2	19.2
89	−5.6	10.5	0.4	13.1	17.7	18.7	−7.0	12.7	14.1	17.1
90	−1.6	14.7	4.3	16.8	20.9	22.0	−1.8	17.1	17.5	20.6
91	−5.8	10.5	0.3	13.0	17.6	18.7	−7.1	12.8	14.0	17.1
92	−1.4	14.8	4.4	17.0	21.1	22.1	−1.6	17.2	17.7	20.5
93	−1.6	13.9	4.0	16.2	21.0	22.0	−2.3	16.4	17.5	20.6
94	−1.4	14.0	4.2	16.3	21.2	22.1	−2.1	16.5	17.5	20.4
95	−1.8	15.2	3.6	17.1	21.0	22.1	−3.4	16.9	17.1	20.1
96	−0.6	15.7	5.4	18.0	22.0	23.1	−0.7	18.2	18.7	21.7
97	−1.6	15.6	3.7	17.4	21.3	22.4	−3.3	17.4	17.4	20.5
98	3.6	15.7	6.9	17.0	24.2	25.3	2.1	16.6	21.2	23.3
99	0.0	15.5	5.2	17.5	21.5	22.6	−1.2	17.3	18.2	21.1
100	−0.3	15.4	5.1	17.6	22.4	23.4	−1.3	17.7	18.8	22.0
101	2.6	16.2	6.7	18.1	21.8	22.8	1.3	17.5	18.3	21.4
102	−0.6	15.7	5.4	18.0	22.1	23.2	−1.0	18.0	18.6	21.7
103	−0.7	16.9	4.7	18.6	22.2	23.4	−2.1	18.8	18.5	21.9

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Table 20 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
104	−0.4	15.7	5.5	18.0	22.3	23.2	−0.8	18.0	18.6	21.6
105	−0.2	14.5	5.5	17.2	22.1	23.1	−0.7	16.8	18.5	21.4
106	−0.1	15.5	5.4	17.7	22.6	23.5	−1.1	17.8	19.0	21.8
107	−11.0	11.6	−0.4	17.0	19.4	24.0	−33.9	11.4	14.2	21.5
108	−14.7	2.5	−4.0	10.7	13.7	17.5	−36.3	2.5	8.8	14.7
109	−10.3	13.8	0.2	18.9	20.6	25.6	−33.7	13.1	15.6	22.9
110	−9.8	13.5	−0.2	17.5	18.6	23.3	−31.3	12.7	13.5	20.8
111	−13.0	5.8	−2.7	13.3	15.5	19.9	−35.6	5.4	10.8	17.1
112	−9.2	15.8	1.4	20.7	22.0	27.0	−33.1	14.7	16.7	24.5
113	−9.4	13.8	0.3	17.9	19.0	23.7	−31.0	13.0	14.1	21.4
114	−12.2	7.5	−2.0	14.6	16.7	21.3	−35.2	6.9	11.8	18.3
115	−8.7	16.2	1.8	21.1	22.4	27.5	−32.7	15.1	17.2	24.8
116	−9.0	14.1	0.5	18.2	19.4	24.1	−31.0	13.1	14.4	21.6
117	−12.0	7.9	−1.8	15.0	16.9	21.6	−35.1	7.2	12.1	18.8
118	−3.5	14.0	1.1	17.9	23.1	28.5	−15.1	13.1	21.8	25.8
119	−0.2	16.5	3.8	17.6	20.1	26.0	−11.7	13.5	20.0	23.5
120	−5.9	9.8	−1.7	14.7	20.6	26.0	−17.0	9.3	19.4	23.0
121	−1.3	16.3	3.8	17.8	20.6	26.3	−12.5	14.2	20.5	24.1
122	−0.5	17.6	3.6	21.1	25.2	31.4	−13.4	16.7	24.7	28.7
123	−0.3	18.1	4.0	19.6	21.4	27.7	−11.9	14.8	21.5	25.2
124	−2.5	15.2	1.8	18.8	24.2	29.8	−15.9	14.7	22.9	26.9
125	1.4	21.3	6.2	22.0	23.7	29.8	−9.4	18.6	23.4	27.5
126	−0.2	18.1	4.5	19.2	21.4	27.5	−11.2	15.5	21.5	24.7
127	−0.4	19.2	4.6	22.6	27.0	33.2	−13.2	18.3	25.9	30.4
128	−24.6	10.0	−6.2	15.2	13.1	18.9	−27.9	10.2	11.9	17.7
129	−25.6	6.0	−7.8	11.7	9.8	15.2	−28.1	6.7	9.0	14.2
130	−23.5	11.1	−5.6	16.1	13.8	20.1	−27.1	11.2	12.9	18.9
131	−23.3	10.1	−6.5	14.9	12.3	18.3	−26.7	10.3	11.5	17.1
132	−24.6	7.2	−7.0	12.9	10.8	16.6	−27.4	7.8	10.2	15.5
133	−23.6	12.5	−5.6	17.2	14.3	21.1	−27.7	12.2	13.5	19.9
134	−23.4	10.0	−6.6	14.9	12.0	18.3	−26.8	10.2	11.8	17.7
135	−24.1	8.0	−6.9	13.5	11.0	17.2	−27.4	8.4	10.8	16.3

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Table 20 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
136	−23.0	13.1	−4.9	17.7	14.9	21.6	−27.2	12.7	14.1	20.4
137	−22.9	10.6	−6.2	15.4	12.5	18.9	−26.5	10.6	12.3	18.2
138	−23.7	8.7	−6.5	14.1	11.5	17.8	−27.2	9.0	11.3	16.8
139	−4.2	15.8	5.3	20.4	21.8	26.2	−25.1	16.8	18.4	24.7
140	−2.4	19.8	7.1	24.2	24.5	29.4	−24.1	20.3	21.1	28.0
141	−2.8	17.7	5.8	21.2	21.3	25.7	−22.8	18.1	18.2	24.5
142	−37.2	−10.7	−26.2	−2.2	10.1	12.3	−38.4	−7.4	1.2	7.5
143	−35.8	−11.8	−25.5	−3.0	9.1	11.3	−35.7	−7.2	0.3	6.0
144	−34.9	−11.9	−25.4	−3.1	9.0	11.4	−35.1	−7.2	0.6	6.3
145	−36.6	−11.7	−25.2	−2.7	9.5	11.7	−37.2	−8.0	1.7	7.4
146	−35.2	−12.7	−24.5	−3.5	8.7	10.7	−34.7	−7.8	0.5	5.9
147	−35.7	−13.3	−24.8	−3.6	8.6	10.9	−34.8	−7.8	0.8	6.3
148	−12.1	−4.6	9.3	12.3	4.9	8.0	−60.9	−24.3	−12.2	−3.6
149	−17.7	−3.2	3.8	8.4	−0.8	3.8	−82.9	−29.1	−19.6	−6.3
150	−31.9	−9.5	−23.3	−2.1	8.4	11.5	−34.1	−5.4	1.6	6.8
151	−8.5	20.5	−8.5	20.6	21.8	27.8	−17.5	18.8	18.1	25.8
152	−9.0	4.7	−1.4	12.2	9.3	13.5	−24.0	3.7	7.7	11.5
153	4.7	23.3	6.9	22.8	18.7	24.3	−14.8	15.3	17.5	22.5
154	−16.4	−2.1	−3.6	8.8	10.6	14.1	−31.1	−1.2	5.4	10.1
155	−7.8	10.9	0.4	16.6	16.0	20.6	−21.4	10.1	13.8	18.3
156	−0.9	18.8	6.7	21.3	18.7	23.6	−21.6	15.6	15.6	21.8
157	−3.6	16.8	2.3	18.9	19.7	25.0	−19.0	13.5	17.7	22.6
158	−12.0	−4.5	9.3	12.3	5.5	8.6	−60.8	−24.2	−11.6	−3.1
159	−12.1	−4.5	9.2	12.1	5.3	8.4	−61.1	−24.4	−11.8	−3.2
160	−31.5	−9.1	−23.0	−1.9	9.0	12.1	−33.9	−5.3	2.1	7.3
161	−5.7	24.0	−5.9	23.8	24.6	30.5	−12.8	24.0	20.7	28.6
162	−12.2	−0.4	−3.4	9.7	8.5	12.1	−23.8	−1.7	5.8	9.1
163	3.3	23.0	7.4	24.0	20.0	26.2	−16.5	18.1	19.9	25.2
164	−18.9	−4.5	−7.3	6.1	8.9	11.8	−30.2	−3.4	3.7	8.0
165	−12.6	−0.1	−2.8	10.2	10.1	13.6	−24.2	0.1	6.6	10.1
166	−4.6	18.3	5.3	21.2	21.2	26.5	−26.6	15.5	17.1	24.4
167	−10.5	9.5	−1.1	16.1	16.3	21.2	−25.1	7.0	13.9	18.6

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Table 20 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
168	−11.9	−4.3	9.5	12.4	5.8	9.0	−60.9	−24.0	−11.4	−2.8
169	−11.9	−4.1	9.5	12.6	5.9	9.0	−61.3	−24.0	−11.4	−2.8
170	−32.3	−10.1	−23.6	−2.8	7.3	10.6	−34.1	−5.9	0.6	5.6
171	−29.4	−0.5	−23.7	4.3	11.6	16.1	−35.7	0.8	4.9	12.2
172	−8.0	5.8	2.2	16.3	11.8	16.4	−24.4	4.5	9.9	14.1
173	−1.7	20.0	4.5	23.3	19.6	25.5	−21.9	17.3	18.1	23.9
174	−13.6	−1.5	−3.9	9.2	9.6	13.1	−25.0	−1.0	6.4	9.7
175	−10.5	14.5	1.7	19.9	20.3	25.7	−32.2	13.1	15.6	23.1
176	−6.5	15.4	3.7	20.7	20.7	26.6	−24.4	16.3	18.3	24.8
177	−11.4	−3.9	9.9	12.8	6.3	9.5	−60.1	−23.6	−10.8	−2.2
178	−12.0	6.2	9.1	14.6	5.7	11.0	−80.5	−14.3	−13.5	2.5
179	−32.0	−9.8	−23.3	−2.5	7.6	10.9	−33.8	−5.7	0.9	5.5
180	−32.3	−9.8	−23.8	−2.6	8.3	11.6	−34.8	−6.1	1.4	6.4
181	−6.1	12.6	3.1	20.8	16.0	21.9	−25.3	10.7	14.9	20.0
182	−5.0	14.6	3.9	22.2	17.2	23.3	−24.5	12.7	16.3	21.7
183	−17.8	−3.5	−6.3	7.0	9.9	12.8	−29.1	−2.7	4.7	8.8
184	−13.1	−1.1	−3.4	9.5	10.0	13.5	−24.4	−0.6	6.7	10.2
185	−11.0	11.1	1.1	18.5	18.7	23.8	−32.0	10.5	13.9	21.0
186	−10.0	8.3	0.8	16.8	16.8	22.0	−26.0	10.1	13.8	19.7
187	−11.1	3.0	13.0	17.4	9.2	13.7	−72.9	−18.5	−10.3	2.9
188	−29.2	2.4	−22.6	6.7	15.2	19.7	−36.3	1.9	7.8	15.2
189	−6.9	14.0	2.9	22.6	17.6	23.4	−27.7	10.9	15.5	21.1
190	−13.2	10.6	−0.4	18.5	19.7	24.4	−35.8	8.7	13.6	20.9
191	−11.9	7.9	−0.7	17.1	17.7	22.5	−29.7	7.7	13.5	19.6
192	−9.8	6.4	14.8	20.0	11.5	16.5	−74.5	−13.7	−8.3	6.3
193	−30.0	2.3	−23.6	6.9	15.3	20.1	−37.7	2.2	7.7	15.3
194	−6.3	15.9	3.7	24.7	19.0	25.5	−28.0	12.6	17.0	23.0
195	−14.2	11.0	−0.1	19.2	20.0	25.1	−37.9	9.0	13.9	21.6
196	−12.7	8.3	−0.4	18.0	18.1	23.3	−31.7	8.7	14.0	20.4
197	−10.4	5.6	14.0	18.9	11.2	15.9	−76.6	−9.4	−8.2	6.5
198	−24.7	11.7	−21.2	11.9	18.3	23.2	−31.9	12.1	11.8	20.2
199	−1.0	23.1	4.4	26.2	22.9	29.2	−22.8	20.7	21.7	28.1

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Table 20 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
200	−5.4	23.4	4.2	25.5	25.6	31.1	−30.1	22.2	20.7	29.0
201	−7.1	21.3	1.7	24.8	25.1	31.1	−23.4	20.4	22.3	28.8
202	−10.7	1.8	12.2	16.5	8.3	12.5	−65.4	−20.3	−10.4	1.6
203	−34.3	−5.2	−26.3	1.1	10.7	14.7	−38.8	−3.0	3.1	9.9
204	−11.6	5.1	−1.7	15.0	12.2	16.9	−27.3	2.5	9.2	13.8
205	−16.9	2.0	−3.5	12.3	14.1	18.0	−35.2	1.4	8.0	13.9
206	−15.9	−0.6	−3.7	10.7	12.4	16.3	−30.8	0.5	8.1	13.0
207	−13.5	0.7	10.8	15.1	6.9	11.3	−74.8	−14.0	−11.4	1.7
208	−24.6	7.9	−20.7	8.4	14.6	18.9	−28.8	10.0	8.5	15.6
209	−5.0	14.9	2.4	20.4	17.0	22.3	−24.1	14.2	15.7	20.9
210	−10.9	12.3	−0.5	16.9	17.7	22.3	−31.9	12.6	13.1	20.1
211	−5.2	13.9	2.1	17.6	17.9	22.5	−20.1	16.3	15.0	21.0
212	−12.2	−1.5	10.1	13.9	6.2	9.8	−65.9	−23.4	−12.3	−1.9
213	−34.4	−8.5	−26.6	−1.5	8.9	12.5	−38.4	−5.6	1.6	7.7
214	−10.8	6.9	1.1	17.8	13.5	18.6	−28.7	6.0	11.5	16.3
215	−19.9	−3.4	−5.8	8.4	11.0	14.7	−37.6	−3.2	5.8	11.0
216	−17.1	0.0	−4.5	11.5	11.5	15.5	−31.0	−0.3	8.0	12.1
217	−12.2	0.3	11.7	15.9	7.4	11.5	−70.8	−20.6	−11.6	0.0
218	−36.2	−6.8	−28.3	−0.1	9.5	13.8	−41.1	−4.0	2.0	8.9
219	−9.7	10.1	1.5	20.2	15.1	20.6	−28.9	9.1	13.0	18.3
220	−17.2	3.2	−4.2	13.7	14.8	18.6	−34.7	2.2	9.1	15.1
221	−17.7	4.0	−4.1	15.0	15.5	20.4	−31.0	4.0	12.2	16.9
222	−9.6	8.0	14.0	18.9	11.4	16.1	−73.1	−2.6	−8.1	7.2
223	−35.0	−5.8	−27.6	0.6	10.3	14.7	−40.5	−3.6	2.9	10.2
224	−4.3	18.1	2.3	22.0	20.1	25.9	−24.7	17.5	18.3	24.3
225	−17.3	0.9	−4.9	11.1	13.3	17.1	−33.7	−0.6	7.6	13.1
226	−15.0	3.7	−2.7	14.4	15.5	20.3	−32.3	5.0	11.4	17.4
227	−13.6	−2.8	9.5	13.1	4.6	8.1	−70.9	−23.5	−13.7	−3.4
228	−33.0	−11.1	−25.9	−4.4	5.7	8.8	−35.7	−7.5	−0.5	4.6
229	−14.4	1.9	−4.3	11.5	8.9	12.8	−29.9	0.4	5.8	10.3
230	−18.9	−3.6	−8.8	5.0	7.8	10.4	−29.9	−4.1	2.5	6.5
231	−17.1	−5.4	−3.4	6.9	7.2	10.8	−28.9	−2.4	4.0	8.1

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Table 20 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
232	−12.5	−1.4	10.6	14.2	6.0	9.6	−70.7	−21.8	−12.4	−1.8
233	−33.5	−5.3	−25.8	0.8	10.2	14.3	−37.9	−2.5	3.6	9.7
234	−8.8	10.2	2.2	20.3	14.8	19.9	−28.0	9.5	13.0	18.0
235	−20.1	−0.7	−8.0	9.4	12.5	16.0	−37.0	−0.9	7.3	13.0
236	−15.6	0.0	−4.7	10.6	9.7	13.7	−28.4	−1.2	6.6	10.1
MAXD	−37.2	44.6	−28.3	47.4	44.5	56.1	−82.9	42.5	47.3	53.5
MD	−10.7	11.4	0.8	17.5	17.4	22.0	−28.6	8.5	11.8	18.4
MAD	13.5	13.5	9.6	17.8	17.4	22.0	30.1	15.1	15.5	18.7

Table 21: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the X3LYP functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−26.5	19.4	−13.0	19.8	18.2	23.8	−22.4	18.9	16.0	22.5
2	−31.9	19.6	−16.3	20.3	18.4	24.6	−26.5	20.1	16.1	23.7
3	−28.4	17.6	−14.9	18.1	17.3	23.0	−24.1	17.7	14.9	21.9
4	−32.7	20.6	−16.8	21.1	19.2	25.6	−27.3	21.1	16.8	24.7
5	−30.3	19.5	−16.0	19.8	18.6	24.7	−25.9	19.3	16.4	23.6
6	−32.8	21.0	−17.0	21.5	19.6	26.1	−27.7	21.4	17.4	25.2
7	−30.1	19.7	−15.8	19.9	18.9	24.9	−25.9	19.4	16.5	23.9
8	−6.9	13.6	16.9	22.7	14.9	19.1	−80.0	−6.4	−10.5	8.4
9	−6.7	15.1	17.7	23.9	16.1	20.5	−82.1	−2.8	−10.0	10.0
10	−17.2	−2.6	10.9	15.5	9.9	13.3	−81.9	−20.0	−15.3	0.0
11	−15.0	0.3	11.9	16.7	11.4	14.8	−81.6	−16.3	−13.8	2.0
12	−6.4	14.3	17.3	23.2	15.6	19.9	−80.0	−5.7	−10.0	9.2
13	−5.0	17.0	19.3	25.7	17.8	22.4	−80.7	−1.1	−8.0	12.5
14	−16.8	−2.1	11.1	15.8	10.1	13.6	−81.7	−19.7	−14.6	0.4
15	−13.2	4.6	14.2	19.4	13.9	17.6	−82.7	−10.4	−11.4	5.7
16	−3.9	18.6	19.9	26.3	18.6	23.2	−79.9	−1.3	−7.1	13.1
17	−4.7	17.5	19.6	26.2	18.3	22.8	−80.5	−0.7	−7.4	13.1

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Table 21 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
18	−16.2	−0.9	11.8	16.9	10.9	14.5	−81.4	−18.5	−14.1	1.9
19	−12.5	6.0	14.8	20.4	14.5	18.4	−82.8	−8.7	−11.5	6.3
20	−3.6	19.1	20.3	26.7	19.0	23.6	−79.9	−1.0	−6.7	13.6
21	8.6	30.3	14.3	30.6	32.8	34.8	4.7	29.8	29.2	32.5
22	−8.6	6.9	−0.7	12.8	18.6	19.8	−9.6	10.7	15.0	17.8
23	8.8	31.4	14.8	32.1	34.8	36.7	5.5	30.7	30.5	34.6
24	6.9	29.4	13.0	30.2	32.5	34.1	3.2	28.8	28.3	32.0
25	6.9	30.4	13.2	31.0	33.3	35.1	2.9	29.6	29.1	33.0
26	7.5	29.0	13.2	29.5	32.1	33.9	3.9	28.3	28.2	32.7
27	8.4	30.1	13.9	30.1	32.8	34.7	4.3	29.2	28.8	32.7
28	10.4	32.2	15.7	32.0	34.1	36.1	6.6	31.2	30.4	34.3
29	9.3	32.1	15.3	32.7	35.4	37.3	6.0	31.3	31.0	34.9
30	9.2	34.3	15.8	34.3	36.2	38.2	5.7	33.2	32.0	36.3
31	−1.5	18.0	6.2	21.8	27.1	28.6	−3.2	20.6	23.1	26.3
32	8.2	33.8	14.8	34.0	35.9	37.9	4.4	33.0	31.6	36.2
33	11.6	33.4	16.8	33.3	35.4	37.6	7.6	32.0	31.2	35.8
34	11.1	32.9	16.3	32.6	34.8	36.7	7.0	31.6	31.3	34.7
35	10.7	33.6	16.6	34.2	36.9	38.9	7.1	32.7	32.8	36.8
36	10.5	36.6	17.2	36.8	38.6	40.6	6.6	35.8	34.6	38.8
37	13.1	34.9	18.2	34.7	36.9	39.1	9.1	33.4	33.1	36.8
38	−2.0	29.5	6.4	27.5	27.9	33.0	−28.9	24.0	21.6	32.9
39	−2.1	31.0	8.8	30.5	29.5	35.0	−32.2	26.9	22.2	31.6
40	−2.0	29.9	6.7	28.1	28.7	34.0	−29.4	24.2	21.8	33.7
41	−1.9	33.1	9.2	32.6	31.5	37.1	−33.1	28.8	24.3	33.9
42	−1.4	30.5	7.2	28.7	29.4	34.8	−29.3	24.5	22.5	34.3
43	−1.2	34.4	9.9	33.8	32.5	38.3	−32.8	29.9	25.1	35.0
44	−1.6	30.5	6.9	28.5	29.3	34.7	−29.5	24.4	22.7	34.5
45	5.3	35.1	12.7	36.7	37.9	45.6	−13.2	30.3	37.1	43.1
46	−13.8	0.9	−8.8	7.0	15.4	19.4	−27.9	−0.9	12.6	16.4
47	−2.6	21.6	4.3	22.0	24.6	30.7	−16.5	16.9	22.9	27.6
48	4.7	39.1	13.4	41.5	41.5	50.4	−14.3	34.6	41.0	48.0
49	−14.0	9.3	−5.9	15.2	22.0	27.3	−27.5	7.7	19.8	24.6

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Table 21 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
50	−4.4	22.6	4.2	23.2	25.9	32.5	−19.7	18.3	24.2	29.4
51	4.0	33.6	12.0	34.9	37.0	44.6	−13.3	29.0	35.9	42.0
52	5.3	41.6	14.6	43.9	43.5	53.0	−13.5	37.2	43.3	51.1
53	−13.2	12.5	−4.4	17.9	24.6	30.3	−27.4	10.9	22.2	27.5
54	−4.6	23.8	4.7	24.4	27.0	33.9	−19.9	19.5	25.5	30.8
55	5.2	35.1	13.2	36.2	37.5	45.0	−11.1	30.0	36.9	42.7
56	−18.4	22.5	−1.9	23.8	18.8	25.0	−25.8	17.9	16.9	23.4
57	−23.3	24.3	−4.5	25.8	19.8	27.0	−30.4	20.2	18.2	25.6
58	−18.6	22.4	−2.3	23.4	18.6	25.1	−26.0	17.7	16.8	23.6
59	−20.1	25.4	−3.9	25.2	19.1	26.3	−29.8	19.8	17.3	25.2
60	−18.6	22.4	−2.5	23.3	18.7	25.3	−26.2	17.5	16.8	23.6
61	−23.8	26.9	−4.4	28.2	21.8	29.5	−31.3	22.7	20.3	28.2
62	−18.6	22.4	−2.5	23.3	18.7	25.3	−26.3	17.5	17.2	23.8
63	6.1	38.7	15.4	37.3	34.7	40.2	−23.1	36.0	29.6	38.6
64	−46.6	0.1	−28.7	5.7	10.8	15.2	−37.5	6.1	7.6	13.7
65	−45.2	−4.6	−28.7	1.7	7.5	11.6	−35.6	2.4	5.1	10.6
66	−45.8	1.6	−28.5	6.7	11.7	16.3	−37.4	7.1	8.6	15.4
67	−43.6	0.4	−28.1	5.4	9.4	13.9	−36.0	5.9	6.9	13.2
68	−44.7	−3.4	−28.4	2.8	8.4	12.8	−35.6	3.4	6.1	11.9
69	−45.9	2.1	−29.1	7.0	11.6	16.4	−38.2	7.3	9.2	15.6
70	−44.4	0.2	−28.6	5.2	9.2	13.9	−36.8	5.7	7.5	13.2
71	−44.5	−3.1	−28.7	2.8	8.4	12.9	−36.0	3.3	6.4	12.1
72	−45.4	2.6	−28.7	7.5	12.1	17.0	−37.8	7.8	8.6	15.8
73	−43.8	0.7	−28.3	5.6	9.6	14.4	−36.6	5.9	7.7	13.5
74	−44.6	−2.9	−28.8	3.0	8.5	13.1	−36.1	3.4	6.0	11.9
75	−16.9	−1.7	11.7	16.2	11.6	14.9	−87.2	−19.9	−13.5	1.5
76	−14.3	2.5	13.2	18.4	13.6	17.2	−85.2	−16.4	−11.5	4.7
77	−15.3	1.4	11.1	16.2	11.5	15.1	−84.1	−16.3	−12.7	3.0
78	−15.8	−0.4	12.2	16.8	12.4	15.7	−86.1	−18.8	−12.4	2.5
79	−14.0	3.6	13.5	19.2	14.0	17.9	−85.1	−15.2	−11.3	5.4
80	−13.9	2.9	12.2	17.4	12.7	16.3	−82.6	−14.8	−11.4	4.5
81	−15.6	0.3	12.2	17.2	12.5	16.0	−86.0	−18.0	−12.4	3.2

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Table 21 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
82	−13.2	4.4	14.2	19.9	14.8	18.7	−84.3	−14.3	−10.5	6.4
83	−13.9	3.0	12.6	18.0	13.2	16.8	−83.3	−15.2	−11.1	5.1
84	−14.7	1.2	12.9	18.0	13.3	16.9	−85.1	−17.2	−11.2	4.3
85	−11.4	8.8	−3.2	11.9	18.1	18.8	−14.2	10.7	13.4	16.1
86	−7.2	12.2	0.8	15.3	21.3	22.1	−9.5	14.1	16.7	19.5
87	−3.3	11.6	2.0	13.8	23.0	23.8	−6.1	11.8	18.4	21.4
88	−7.1	11.4	0.8	14.6	20.9	21.6	−8.9	13.2	16.1	19.1
89	−10.7	9.5	−2.8	12.3	18.3	19.1	−13.8	11.0	13.4	16.7
90	−7.1	13.2	0.9	15.9	21.2	22.0	−8.9	14.9	16.5	19.6
91	−10.7	9.6	−2.9	12.3	18.2	19.1	−13.8	11.1	13.5	16.7
92	−6.9	13.4	1.0	16.0	21.3	22.2	−8.7	15.0	16.7	19.8
93	−6.4	13.1	1.3	15.9	21.9	22.7	−9.0	14.6	17.2	20.0
94	−6.3	13.1	1.4	15.9	22.0	22.7	−8.9	14.6	17.3	20.0
95	−7.4	13.5	−0.6	15.5	20.7	21.5	−10.8	14.5	16.0	19.6
96	−6.1	14.3	1.9	16.9	22.1	23.1	−7.9	16.0	17.4	20.7
97	−7.5	13.7	−0.6	15.7	20.8	21.7	−11.0	14.8	16.1	19.6
98	−1.2	14.0	3.3	15.3	23.9	24.8	−4.4	13.8	19.8	22.3
99	−4.8	14.4	2.2	16.8	22.0	22.9	−7.6	15.4	17.8	20.3
100	−5.3	14.4	2.2	17.1	23.1	23.9	−8.2	15.8	18.6	21.8
101	−1.2	15.7	4.7	18.0	22.9	23.8	−3.9	16.1	18.7	21.6
102	−6.2	14.1	1.8	16.8	22.2	23.1	−8.2	15.6	17.8	20.8
103	−6.6	15.2	0.4	16.9	21.7	22.7	−9.8	16.2	17.2	20.5
104	−6.1	14.2	2.0	16.8	22.4	23.1	−8.1	15.7	17.8	20.8
105	−4.6	13.9	3.0	16.8	22.9	23.7	−6.7	15.3	18.4	21.6
106	−5.1	14.5	2.5	17.1	23.3	24.0	−7.9	15.8	18.8	21.6
107	−17.2	9.2	−4.7	15.0	18.8	22.7	−44.3	8.1	10.7	19.0
108	−20.3	−0.1	−8.4	8.2	12.8	16.0	−45.7	−0.5	5.7	12.1
109	−16.3	11.6	−3.9	17.1	20.3	24.5	−44.0	10.0	12.3	20.7
110	−15.9	11.0	−4.5	15.5	18.0	22.0	−41.4	9.4	10.5	18.8
111	−18.4	3.5	−6.8	11.1	15.0	18.6	−44.8	2.6	7.8	14.8
112	−15.2	13.6	−2.7	18.9	21.7	25.9	−43.4	11.7	13.8	22.5
113	−15.3	11.5	−3.9	15.9	18.5	22.5	−41.0	9.8	10.9	19.1

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Table 21 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
114	−17.8	5.1	−6.3	12.4	16.0	19.9	−44.7	4.0	8.8	15.9
115	−14.8	14.0	−2.4	19.2	22.0	26.2	−43.1	12.0	14.2	22.6
116	−15.1	11.7	−3.8	16.2	18.8	22.8	−41.0	9.8	11.2	19.5
117	−17.6	5.5	−6.2	12.6	16.2	20.1	−44.6	4.2	9.1	16.5
118	−8.7	11.1	−3.0	15.2	22.3	26.8	−24.1	8.9	19.3	24.2
119	−7.3	12.3	−2.1	13.3	17.9	22.7	−22.2	7.9	15.9	20.1
120	−10.8	6.9	−5.8	11.8	19.8	24.3	−25.8	5.4	17.0	21.6
121	−8.9	12.0	−2.4	13.4	18.2	22.9	−23.7	8.4	15.7	20.3
122	−5.8	14.9	−0.6	18.4	24.5	29.6	−22.7	12.5	21.9	26.6
123	−7.5	14.1	−2.1	15.1	19.2	24.4	−22.4	9.3	17.2	21.1
124	−8.9	11.5	−3.5	15.1	22.5	27.2	−26.5	9.6	19.5	24.7
125	−7.4	15.9	−1.2	16.4	20.3	25.3	−21.8	11.7	17.9	23.0
126	−8.2	13.5	−2.2	14.2	18.5	23.6	−22.8	9.3	16.4	20.5
127	−6.9	15.6	−0.5	19.0	25.5	30.6	−23.8	13.3	22.5	27.9
128	−34.5	4.7	−14.1	10.3	10.3	15.2	−38.9	4.5	7.1	13.4
129	−34.8	1.0	−15.1	7.2	7.3	11.9	−38.2	1.5	4.6	10.2
130	−33.3	5.8	−13.9	10.9	10.7	16.0	−38.3	5.3	8.1	14.6
131	−32.9	4.9	−14.7	9.7	9.3	14.3	−37.6	4.5	6.7	13.2
132	−33.7	2.3	−14.5	8.2	8.2	13.1	−37.6	2.5	5.8	11.6
133	−33.5	7.2	−13.8	12.1	11.5	17.1	−38.9	6.4	9.0	15.3
134	−32.9	4.8	−14.7	9.7	9.1	14.3	−37.6	4.5	7.3	13.3
135	−33.3	3.0	−14.6	8.7	8.4	13.6	−37.7	3.0	6.5	12.3
136	−33.1	7.6	−13.3	12.5	11.9	17.6	−38.5	6.8	8.9	15.7
137	−32.5	5.4	−14.4	10.2	9.5	14.8	−37.3	4.8	7.8	14.0
138	−33.1	3.6	−14.3	9.2	8.8	14.2	−37.6	3.5	7.0	13.0
139	−11.6	11.9	−0.2	16.8	19.7	23.5	−36.9	12.1	13.9	21.0
140	−9.6	16.3	1.7	20.8	22.7	26.9	−35.7	15.8	17.1	24.3
141	−9.9	14.0	0.5	17.8	19.4	23.1	−34.1	13.5	14.3	21.0
142	−42.5	−12.5	−30.5	−3.6	10.5	12.3	−44.7	−9.5	0.1	6.6
143	−40.7	−13.6	−29.6	−4.6	9.4	11.2	−41.4	−9.2	−1.1	5.2
144	−39.9	−13.8	−29.4	−4.4	9.6	11.5	−40.7	−9.1	−0.4	5.3
145	−42.0	−13.8	−29.6	−4.4	9.9	11.7	−43.5	−10.4	0.3	6.4

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Table 21 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
146	−40.3	−14.8	−28.8	−5.4	8.8	10.5	−40.6	−10.2	−0.8	4.7
147	−40.8	−15.2	−28.8	−5.0	9.3	11.2	−40.6	−9.8	−0.1	5.8
148	−14.1	−4.9	10.8	14.3	9.1	11.6	−68.5	−25.4	−13.8	−2.9
149	−16.2	1.6	8.8	14.1	6.4	10.2	−89.0	−26.3	−19.3	−2.5
150	−35.2	−9.5	−26.1	−2.1	10.7	13.3	−39.3	−6.0	2.2	7.6
151	−12.6	20.5	−12.0	20.6	23.5	28.3	−23.5	18.2	15.7	24.3
152	−11.8	4.3	−3.4	11.6	10.8	14.2	−30.1	2.5	7.1	11.3
153	1.0	22.4	4.0	21.5	18.9	23.5	−21.7	13.2	15.2	20.6
154	−20.5	−3.7	−6.3	7.7	11.0	14.0	−37.8	−3.1	4.1	9.1
155	−12.3	9.3	−3.4	14.7	15.9	19.7	−29.4	7.2	11.6	16.7
156	−4.1	18.6	4.9	21.3	19.8	23.8	−27.9	14.6	14.2	21.3
157	−9.5	14.2	−2.6	16.1	18.6	23.0	−28.0	9.8	14.4	19.7
158	−14.2	−5.0	10.5	14.0	9.5	12.1	−68.7	−25.4	−13.7	−2.8
159	−14.2	−4.9	10.5	13.9	9.4	11.9	−68.8	−25.5	−13.9	−3.0
160	−34.9	−9.3	−26.1	−2.1	11.1	13.8	−39.3	−6.1	2.3	7.4
161	−10.5	23.4	−10.1	23.2	26.1	30.8	−19.7	22.4	18.1	27.2
162	−15.4	−1.4	−5.9	8.5	9.5	12.5	−29.9	−3.7	5.0	9.1
163	0.0	22.9	5.4	24.0	21.5	26.7	−23.2	16.8	17.8	23.9
164	−22.9	−6.1	−10.2	4.8	9.1	11.5	−36.8	−5.5	1.8	6.9
165	−16.1	−1.6	−5.6	8.8	10.7	13.6	−30.7	−2.4	5.4	8.8
166	−9.3	17.5	2.4	20.5	21.7	26.2	−34.7	13.9	14.7	22.8
167	−15.4	7.9	−5.0	14.2	16.6	20.6	−33.2	4.2	11.6	15.8
168	−14.2	−4.9	10.6	14.1	9.7	12.4	−68.8	−25.3	−13.4	−2.5
169	−14.0	−4.5	10.8	14.4	9.9	12.5	−69.2	−25.1	−13.7	−2.5
170	−35.5	−10.2	−26.3	−2.8	9.7	12.5	−39.1	−6.6	0.7	6.8
171	−32.7	0.4	−26.8	4.9	14.6	18.3	−41.3	0.9	5.0	12.7
172	−10.9	5.3	0.3	16.0	13.8	17.7	−30.8	3.0	9.6	14.1
173	−6.4	18.9	0.9	21.9	20.0	24.9	−31.0	14.7	15.3	21.7
174	−17.1	−3.0	−6.6	7.8	10.2	13.1	−31.4	−3.4	5.0	8.3
175	−16.6	12.5	−2.5	18.1	20.0	24.5	−42.0	10.5	12.1	21.0
176	−12.2	13.4	−0.3	18.9	20.7	25.7	−33.8	13.4	15.2	22.8
177	−13.7	−4.5	11.0	14.5	10.2	12.8	−68.0	−24.9	−13.0	−1.8

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Table 21 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
178	−11.1	11.2	13.6	20.0	12.6	17.0	−88.1	−11.0	−12.6	7.3
179	−35.2	−9.9	−26.0	−2.6	10.0	12.8	−38.9	−6.4	0.9	7.0
180	−35.8	−10.1	−27.0	−3.0	10.4	13.1	−40.3	−7.0	1.3	6.7
181	−10.3	11.7	0.0	19.7	17.4	22.3	−33.6	8.6	12.9	19.1
182	−9.3	13.7	0.7	21.1	18.5	23.6	−33.0	10.5	14.4	20.8
183	−21.9	−5.2	−9.3	5.6	10.0	12.4	−35.8	−4.9	2.7	8.0
184	−16.6	−2.6	−6.2	8.1	10.5	13.4	−30.8	−3.0	5.3	9.6
185	−16.4	9.4	−2.6	16.9	18.8	23.0	−41.0	8.1	11.2	19.4
186	−14.9	6.4	−2.8	15.1	17.1	21.4	−34.5	7.4	11.7	18.4
187	−15.2	1.8	13.2	18.4	12.5	16.2	−84.7	−21.2	−13.9	2.6
188	−35.1	0.5	−27.5	5.3	16.5	20.3	−44.4	−0.8	6.3	14.6
189	−11.8	12.3	−0.2	21.7	19.1	23.9	−36.6	7.9	13.9	19.7
190	−20.1	7.1	−4.9	16.0	18.9	22.9	−46.5	4.5	10.2	18.3
191	−17.8	4.7	−4.9	14.6	17.4	21.5	−39.3	3.7	10.8	17.4
192	−14.1	5.5	15.1	21.1	14.8	18.9	−86.9	−16.2	−12.2	6.0
193	−36.5	0.1	−29.4	5.0	16.0	20.0	−46.5	−0.7	5.9	14.1
194	−12.0	13.6	−0.1	23.1	19.8	25.2	−37.9	9.1	14.8	21.1
195	−21.2	7.7	−4.6	17.0	19.4	23.7	−48.7	5.1	10.6	19.1
196	−18.9	5.2	−4.5	15.8	18.0	22.4	−41.5	4.9	11.5	18.5
197	−11.8	8.1	16.3	22.1	16.9	20.8	−86.5	−7.9	−9.3	9.1
198	−30.3	11.1	−26.3	11.1	19.7	23.6	−40.4	10.3	10.1	19.1
199	−6.7	21.5	0.3	24.8	23.4	28.7	−33.3	17.5	18.8	26.0
200	−11.5	21.7	0.7	24.5	25.8	30.4	−40.7	19.4	17.8	27.2
201	−14.7	18.1	−4.1	21.8	24.0	29.0	−34.9	15.8	18.6	25.7
202	−14.7	0.1	11.7	16.7	10.7	14.2	−76.2	−23.5	−15.1	−0.4
203	−39.2	−6.3	−30.9	−0.1	12.5	15.8	−45.9	−4.8	2.4	9.8
204	−15.6	3.6	−4.8	13.7	13.3	17.2	−34.6	0.0	7.7	12.8
205	−22.3	−0.6	−7.3	10.3	13.9	17.2	−43.8	−1.8	5.2	12.2
206	−21.2	−3.5	−7.7	8.4	12.2	15.5	−39.2	−3.0	5.7	11.3
207	−14.8	2.9	12.9	18.0	12.4	16.0	−84.2	−13.0	−12.5	3.8
208	−29.6	7.4	−25.2	7.6	15.9	19.4	−36.8	8.0	7.1	15.3
209	−9.9	13.5	−1.2	19.0	17.6	22.1	−33.6	11.3	13.4	19.5

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Table 21 – continued from previous page

N	6–31G**		6–311G**		6–311++G(3df,2p)		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
210	−16.1	10.7	−3.9	15.7	18.0	21.8	−41.3	10.1	10.8	18.7
211	−9.6	12.5	−1.0	16.4	18.3	22.1	−28.5	13.5	13.3	19.9
212	−16.1	−3.2	9.9	14.3	8.8	11.8	−76.2	−26.4	−16.3	−3.1
213	−38.3	−9.0	−30.0	−1.8	11.5	14.6	−44.4	−6.8	1.7	8.1
214	−14.3	6.3	−1.1	17.5	15.9	20.2	−36.2	4.1	10.6	16.0
215	−24.2	−5.0	−8.3	7.5	12.2	15.3	−45.0	−5.3	4.2	10.2
216	−21.6	−2.0	−7.7	10.1	12.6	16.0	−38.6	−3.3	6.6	11.0
217	−15.9	−0.9	11.9	16.9	10.7	14.0	−81.7	−22.9	−15.2	−0.7
218	−40.7	−7.4	−32.4	−0.5	12.0	15.6	−47.9	−5.4	2.1	9.4
219	−13.3	9.6	−0.5	20.2	17.6	22.2	−36.8	7.1	12.6	17.9
220	−22.1	1.4	−7.5	12.4	15.3	18.6	−42.9	−0.4	7.2	13.7
221	−23.9	0.9	−8.9	12.3	15.4	19.5	−40.6	−0.1	9.6	14.1
222	−10.8	11.0	16.4	22.2	17.0	20.9	−83.2	−1.0	−9.1	9.6
223	−39.5	−6.5	−31.7	0.0	12.8	16.4	−47.2	−5.0	3.0	10.3
224	−10.3	16.1	−2.5	19.7	19.8	24.6	−35.5	14.0	15.2	22.8
225	−21.9	−1.2	−8.1	9.6	13.7	16.8	−41.1	−3.2	5.5	11.6
226	−19.9	1.5	−6.3	12.6	16.0	20.0	−41.0	1.9	10.1	16.5
227	−17.3	−4.1	10.0	14.2	7.9	10.9	−81.4	−25.8	−17.1	−4.0
228	−36.3	−11.4	−28.7	−4.6	8.1	10.8	−40.7	−8.5	−0.2	5.1
229	−18.2	0.7	−6.9	10.5	10.4	13.6	−36.9	−1.7	4.7	9.3
230	−23.9	−6.3	−12.5	2.8	6.9	9.0	−36.6	−6.9	−0.3	5.1
231	−20.1	−6.5	−4.5	7.0	9.6	12.7	−34.1	−3.7	4.3	9.2
232	−16.2	−2.6	10.9	15.2	9.3	12.3	−81.4	−24.0	−15.8	−2.3
233	−38.2	−6.2	−29.8	0.3	12.6	16.0	−44.7	−3.9	3.3	10.6
234	−12.6	9.4	0.0	20.0	17.1	21.4	−36.0	7.5	12.6	18.4
235	−25.2	−2.7	−11.6	7.8	12.9	15.8	−45.3	−3.7	4.9	11.2
236	−20.2	−2.4	−7.8	8.9	10.5	13.9	−35.2	−4.1	5.3	9.1
MAXD	−46.6	41.6	−32.4	43.9	43.5	53.0	−89.0	37.2	43.3	51.1
MD	−15.9	9.8	−2.5	16.2	18.0	21.8	−37.2	5.9	9.5	17.1
MAD	17.3	12.3	10.9	16.6	18.0	21.8	37.9	13.1	13.8	17.4

Table 22: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the B2GP-PLYP functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−37.1	38.2	−28.4	38.2	−34.3	38.4	−4.4	36.7
2	−43.3	42.4	−32.8	42.8	−39.4	43.5	−5.6	41.2
3	−38.6	39.6	−29.8	39.7	−35.6	40.2	−5.2	38.9
4	−44.7	46.5	−34.0	46.7	−40.8	47.6	−6.0	45.2
5	−41.7	44.9	−32.4	44.8	−38.7	45.4	−5.6	43.9
6	−45.2	49.9	−34.7	50.2	−41.6	50.9	−6.0	48.7
7	−41.8	48.0	−32.6	48.0	−39.0	48.4	−6.0	47.0
8	−8.0	37.2	7.7	43.0	−76.2	17.7	−19.0	23.7
9	−8.8	41.5	7.6	47.3	−79.3	23.8	−18.9	28.6
10	−17.5	21.0	4.9	35.8	−77.3	3.3	−19.5	17.2
11	−15.5	23.8	5.3	37.0	−77.2	6.8	−19.0	18.9
12	−8.3	40.7	7.3	46.4	−77.1	21.2	−18.8	27.6
13	−7.6	46.3	8.7	51.9	−78.4	28.3	−17.7	33.3
14	−17.5	24.4	4.7	39.1	−77.5	6.5	−19.5	20.5
15	−15.2	31.0	5.5	42.9	−79.9	15.4	−19.2	25.0
16	−7.3	47.9	7.3	52.0	−78.7	28.2	−18.6	33.7
17	−7.8	49.6	8.4	55.2	−78.8	31.5	−18.0	36.7
18	−17.5	28.3	4.7	42.9	−77.8	10.5	−19.3	24.6
19	−15.3	35.4	5.2	46.8	−80.8	20.0	−19.8	28.9
20	−7.3	51.3	7.1	55.3	−79.2	31.4	−18.8	37.0
21	−10.6	47.2	−10.3	44.9	−15.8	46.7	0.3	41.5
22	−18.1	24.8	−13.8	28.2	−19.5	28.3	−1.1	29.0
23	−12.7	51.0	−12.0	49.1	−17.6	50.4	−0.5	46.1
24	−12.6	49.7	−11.6	48.0	−17.5	49.2	−0.8	44.5
25	−13.6	50.8	−12.5	48.9	−18.9	50.1	−1.0	45.5
26	−11.9	48.7	−10.9	46.9	−16.6	48.1	−0.5	43.8
27	−11.2	49.9	−10.9	47.5	−16.5	49.1	−0.2	44.4
28	−10.3	51.4	−10.1	48.8	−15.4	50.7	0.3	45.5

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Table 22 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
29	−12.9	54.6	−12.3	52.6	−17.8	53.9	−0.8	49.5
30	−13.6	57.2	−12.5	54.7	−18.6	56.3	−0.7	51.0
31	−18.0	40.9	−14.7	42.3	−20.7	43.4	−1.3	41.9
32	−14.7	56.8	−13.4	54.5	−20.0	56.1	−1.5	50.9
33	−10.9	55.7	−11.0	53.0	−16.6	54.3	−0.9	49.6
34	−10.1	54.9	−10.1	52.2	−15.4	53.8	0.4	48.9
35	−12.1	59.1	−11.7	57.0	−17.3	58.3	−0.1	54.0
36	−13.5	62.6	−12.4	60.1	−19.0	61.7	0.3	56.4
37	−9.8	59.9	−10.0	57.2	−15.5	58.5	0.2	53.9
38	−25.1	51.5	−20.2	49.4	−50.6	47.3	−9.5	46.3
39	−26.5	57.1	−19.7	56.3	−55.6	54.1	−10.5	51.9
40	−25.8	54.8	−20.7	52.8	−51.9	50.3	−9.6	50.3
41	−28.0	62.3	−21.0	61.5	−58.1	59.1	−10.8	56.9
42	−25.7	58.3	−20.8	56.2	−52.3	53.5	−9.4	53.9
43	−28.2	66.6	−21.4	65.6	−58.7	63.2	−10.8	61.1
44	−26.1	61.0	−21.3	58.9	−52.8	56.2	−9.7	56.6
45	−29.4	70.8	−26.9	71.4	−46.4	67.4	−7.6	71.4
46	−30.0	36.6	−28.3	40.8	−42.3	35.1	−7.8	47.1
47	−23.6	58.0	−20.2	58.0	−35.8	54.6	−5.2	59.3
48	−33.9	79.2	−30.7	80.4	−51.7	76.1	−8.7	79.8
49	−36.4	49.1	−32.3	53.2	−48.2	47.9	−8.9	58.2
50	−27.1	62.8	−22.2	63.2	−40.8	59.8	−5.9	64.8
51	−29.7	72.4	−26.3	72.9	−45.4	69.2	−7.3	73.7
52	−35.7	84.9	−32.3	86.0	−53.4	81.9	−9.4	85.2
53	−38.3	55.5	−33.9	59.3	−50.8	54.5	−9.6	64.2
54	−28.7	67.2	−23.4	67.4	−42.5	64.2	−6.5	69.3
55	−28.9	76.7	−25.5	76.8	−43.7	73.0	−7.2	77.1
56	−32.3	44.0	−19.6	45.7	−37.7	41.4	−6.5	41.0
57	−39.1	49.9	−24.2	52.0	−44.1	47.7	−7.8	46.6
58	−32.8	46.7	−20.3	48.2	−38.2	44.0	−6.8	44.0
59	−35.5	53.7	−23.1	54.1	−42.7	50.1	−8.0	48.8
60	−33.0	49.6	−20.6	51.0	−38.6	46.7	−6.9	46.9

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Table 22 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
61	−41.4	58.9	−26.2	60.9	−46.9	56.7	−8.6	55.5
62	−33.1	52.5	−20.8	54.0	−38.9	49.6	−7.0	49.9
63	−24.2	77.8	−19.0	76.6	−52.4	76.4	−7.9	72.3
64	−51.7	30.7	−38.2	35.6	−43.9	36.9	−7.7	39.3
65	−48.8	26.0	−36.2	31.5	−40.4	33.0	−7.7	35.8
66	−51.7	36.1	−38.7	40.6	−44.5	41.9	−8.1	44.2
67	−47.5	34.6	−36.5	38.6	−41.0	40.0	−6.9	41.7
68	−48.6	31.2	−36.3	36.6	−40.6	38.0	−7.2	41.1
69	−52.5	39.7	−40.1	44.0	−46.0	45.2	−8.7	47.3
70	−48.6	37.6	−37.3	41.7	−42.1	43.2	−7.0	45.0
71	−49.1	34.5	−37.3	39.8	−41.7	41.1	−8.4	44.0
72	−52.1	43.2	−39.8	47.5	−45.7	48.7	−8.6	51.0
73	−48.4	41.0	−37.3	45.0	−42.2	46.3	−6.9	48.4
74	−49.3	37.7	−37.5	43.0	−41.9	44.2	−8.4	47.3
75	−17.2	28.5	6.1	44.0	−82.5	10.4	−19.4	24.9
76	−16.8	36.1	5.2	49.7	−82.7	17.3	−19.6	31.1
77	−16.8	35.2	4.0	47.5	−80.5	17.6	−19.2	29.9
78	−17.0	33.5	5.8	48.4	−82.3	15.2	−18.9	29.5
79	−16.9	40.2	4.8	53.3	−83.1	21.4	−20.2	34.9
80	−15.8	39.8	4.6	51.8	−79.4	22.2	−19.3	34.6
81	−17.3	37.1	5.1	51.7	−82.7	18.8	−19.8	33.1
82	−16.3	43.9	5.3	56.9	−82.5	25.2	−19.7	38.7
83	−16.2	42.9	4.6	55.3	−80.6	24.8	−19.4	38.0
84	−16.5	41.0	5.7	55.4	−82.0	22.6	−19.1	37.0
85	−19.9	37.8	−15.5	39.0	−22.9	39.7	−2.3	39.5
86	−18.5	41.0	−14.6	41.9	−21.1	42.9	−2.6	42.0
87	−17.9	35.1	−15.5	35.9	−21.3	35.5	−1.3	40.4
88	−18.3	40.1	−14.3	41.1	−20.4	41.9	−3.0	41.5
89	−20.0	42.3	−15.8	43.2	−23.3	43.8	−3.4	43.5
90	−18.7	46.0	−14.8	46.5	−20.9	47.7	−2.7	46.0
91	−20.1	42.4	−15.9	43.3	−23.3	43.9	−3.5	43.6
92	−18.5	46.1	−14.6	46.6	−20.7	47.8	−2.5	46.2

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Table 22 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
93	−18.6	45.8	−14.7	46.5	−21.4	47.4	−2.9	46.6
94	−18.5	45.8	−14.7	46.5	−21.4	47.4	−2.6	46.7
95	−17.8	48.8	−14.7	48.9	−21.4	49.9	−2.1	48.5
96	−17.9	50.2	−14.0	50.6	−20.1	51.8	−2.2	50.2
97	−17.9	49.0	−14.8	49.2	−21.7	50.3	−1.8	48.9
98	−16.6	44.3	−15.0	44.1	−20.3	44.3	−0.4	48.2
99	−16.4	49.7	−13.2	50.0	−19.5	50.8	−1.5	49.8
100	−17.9	50.1	−14.2	50.7	−21.0	51.6	−1.7	51.0
101	−14.6	53.5	−12.6	53.8	−17.9	54.2	−2.0	53.3
102	−18.3	52.9	−14.3	53.4	−20.7	54.4	−2.2	53.2
103	−17.8	53.3	−14.7	53.2	−21.4	54.4	−2.0	52.6
104	−18.2	53.0	−14.2	53.5	−20.6	54.5	−2.2	53.2
105	−17.6	52.3	−14.0	53.2	−20.3	53.8	−2.7	53.5
106	−17.8	53.1	−14.2	53.7	−21.0	54.5	−1.4	53.8
107	−33.3	42.2	−24.0	47.2	−58.5	42.0	−11.9	46.5
108	−31.3	33.1	−22.2	40.3	−54.9	33.3	−10.2	40.2
109	−34.2	48.5	−25.0	53.3	−60.0	47.9	−11.9	52.1
110	−31.2	47.5	−23.2	51.1	−55.0	46.7	−11.0	49.9
111	−31.6	40.6	−22.9	47.2	−56.3	40.3	−10.9	46.7
112	−34.4	53.6	−25.3	58.2	−60.8	52.6	−12.2	56.5
113	−31.1	51.2	−23.1	54.7	−55.1	50.3	−10.8	53.6
114	−31.8	45.3	−23.2	51.6	−57.0	44.8	−10.9	51.2
115	−34.1	56.9	−25.1	61.5	−60.6	55.9	−11.3	60.1
116	−31.5	54.4	−23.6	57.9	−55.9	53.3	−11.3	56.7
117	−31.9	48.6	−23.3	54.8	−57.1	48.0	−10.9	54.3
118	−31.1	55.5	−28.9	58.3	−44.8	54.2	−8.7	63.2
119	−23.9	57.2	−21.9	57.6	−37.5	53.9	−5.9	60.8
120	−30.8	51.5	−29.1	54.9	−43.6	50.7	−8.0	60.8
121	−25.7	57.2	−22.7	57.9	−39.2	54.5	−6.6	61.2
122	−29.7	63.1	−28.1	65.5	−45.0	61.6	−7.5	69.8
123	−24.9	63.1	−22.9	63.6	−38.4	59.5	−6.3	66.4
124	−31.5	60.6	−30.1	62.9	−47.4	59.4	−9.0	68.2

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Table 22 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
125	−25.4	65.3	−23.1	65.0	−38.3	62.1	−6.6	67.6
126	−25.3	62.6	−22.7	62.8	−38.4	59.5	−6.7	65.9
127	−32.1	67.4	−29.7	69.7	−47.5	65.9	−8.7	74.3
128	−42.7	37.0	−25.7	42.6	−44.9	38.2	−9.4	41.9
129	−41.4	33.3	−24.7	39.4	−42.6	35.0	−9.4	38.7
130	−41.7	41.9	−25.8	47.0	−44.5	42.9	−8.8	46.6
131	−39.8	40.8	−25.2	45.4	−42.4	41.8	−8.1	45.0
132	−40.9	38.5	−24.7	44.4	−42.6	40.1	−8.8	43.8
133	−43.5	46.6	−27.1	51.6	−46.5	47.4	−10.6	50.7
134	−40.1	43.9	−25.5	48.5	−42.7	44.9	−8.4	47.8
135	−41.2	42.3	−25.4	48.1	−43.4	43.7	−9.8	47.6
136	−43.1	50.0	−26.8	55.1	−46.2	50.8	−9.8	54.3
137	−40.2	47.5	−25.7	52.1	−43.0	48.3	−8.4	51.5
138	−41.2	45.9	−25.5	51.6	−43.5	47.3	−9.8	51.1
139	−29.8	54.7	−21.0	59.5	−53.3	55.8	−9.0	59.5
140	−30.9	66.0	−22.4	70.6	−55.4	66.6	−9.6	69.9
141	−28.0	63.5	−20.7	67.0	−50.8	63.9	−8.7	66.1
142	−47.6	14.1	−39.7	21.2	−50.2	17.6	−12.2	27.7
143	−44.4	7.0	−37.5	14.1	−45.5	11.7	−11.5	20.6
144	−43.1	4.2	−37.0	11.6	−44.4	9.2	−10.2	18.4
145	−46.3	13.5	−38.0	21.0	−48.0	17.3	−11.1	28.0
146	−43.1	6.4	−35.8	13.8	−43.7	11.4	−9.9	20.8
147	−43.1	3.6	−35.7	11.6	−43.2	9.3	−9.3	19.0
148	−13.1	10.3	5.5	24.9	−63.8	−11.0	−17.8	5.2
149	−12.5	25.3	4.1	33.7	−80.6	−2.0	−22.3	12.5
150	−37.3	4.4	−32.9	9.5	−41.1	8.0	−7.3	16.0
151	−25.9	34.5	−29.2	33.4	−36.7	32.8	−6.5	31.9
152	−18.7	20.6	−13.7	26.8	−35.5	19.4	−4.9	23.2
153	−13.5	37.1	−13.7	35.9	−34.7	29.5	−5.3	31.1
154	−28.3	15.5	−17.9	25.2	−44.7	16.5	−9.4	23.1
155	−23.7	30.7	−18.7	35.1	−39.5	29.5	−6.3	33.2
156	−19.6	37.8	−13.9	39.8	−42.7	34.6	−7.2	35.0

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Table 22 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
157	−23.7	34.6	−19.9	36.2	−40.9	31.3	−7.2	35.4
158	−13.5	13.1	5.1	27.6	−64.3	−8.1	−17.6	8.6
159	−13.4	13.2	5.1	27.7	−64.2	−8.0	−17.7	8.6
160	−37.4	7.4	−33.1	12.5	−41.4	10.8	−7.1	19.3
161	−25.5	39.3	−29.1	38.2	−34.6	39.1	−5.7	36.8
162	−21.7	16.8	−16.2	25.1	−34.9	15.1	−6.4	22.2
163	−17.2	41.0	−15.2	41.8	−39.3	35.9	−6.1	37.2
164	−29.8	15.5	−21.4	24.6	−42.6	16.5	−10.3	23.4
165	−23.5	21.9	−17.2	30.5	−36.7	21.9	−7.7	27.7
166	−26.5	40.0	−18.2	42.4	−50.9	37.3	−9.5	39.7
167	−27.6	33.1	−21.6	38.2	−44.2	30.4	−7.2	36.7
168	−13.7	16.9	4.9	31.6	−64.6	−4.3	−17.6	12.7
169	−13.5	17.6	5.1	32.1	−64.9	−3.7	−17.6	13.1
170	−38.3	10.1	−33.8	15.3	−41.5	13.9	−8.7	21.5
171	−37.9	23.3	−36.9	25.9	−46.3	24.2	−8.8	29.8
172	−20.8	29.0	−13.5	38.3	−39.2	27.5	−6.1	32.3
173	−22.1	43.0	−18.5	45.5	−44.8	39.9	−6.6	41.3
174	−24.2	24.2	−18.0	33.1	−37.2	24.5	−7.7	30.9
175	−32.1	40.3	−22.0	44.9	−56.0	39.2	−10.4	42.5
176	−28.6	42.7	−20.8	47.1	−48.5	43.8	−8.5	46.1
177	−13.3	21.2	5.3	35.8	−63.9	0.0	−17.2	17.0
178	−10.7	44.7	5.0	49.8	−82.9	22.7	−20.5	31.3
179	−38.1	14.3	−33.6	19.4	−41.4	18.0	−8.5	25.7
180	−38.6	14.3	−34.3	19.3	−42.7	17.6	−8.3	26.3
181	−24.0	40.3	−17.9	47.2	−45.3	38.1	−7.1	41.9
182	−24.0	42.4	−18.1	48.7	−45.7	40.2	−7.1	43.5
183	−29.1	23.9	−20.9	33.0	−42.0	24.6	−9.6	31.9
184	−23.8	28.3	−17.6	37.2	−36.7	28.7	−7.4	35.1
185	−31.1	41.2	−21.3	47.5	−54.2	40.7	−10.2	44.8
186	−28.1	39.8	−20.3	46.9	−46.0	41.8	−8.0	45.8
187	−17.2	25.5	3.5	37.8	−82.4	1.9	−22.3	18.3
188	−43.1	22.2	−41.2	24.8	−52.3	21.6	−9.9	30.2

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Table 22 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
189	−27.1	37.3	−20.6	45.1	−50.3	34.0	−8.9	38.5
190	−36.5	35.8	−26.7	42.9	−61.6	34.0	−13.4	40.5
191	−32.4	34.9	−24.9	42.6	−52.5	34.8	−11.0	41.1
192	−17.8	32.7	3.5	44.1	−86.3	10.2	−22.8	24.9
193	−44.9	25.4	−43.3	28.2	−54.6	25.2	−11.5	33.5
194	−29.0	42.2	−22.4	50.1	−53.2	38.7	−9.6	43.3
195	−38.9	40.0	−27.3	47.6	−65.1	38.2	−14.2	44.6
196	−34.7	39.3	−25.8	47.8	−55.9	39.9	−11.9	45.7
197	−16.1	39.0	5.0	50.6	−86.5	22.4	−20.6	32.3
198	−42.7	38.2	−42.3	37.6	−52.3	37.9	−10.3	41.5
199	−26.9	51.6	−23.6	54.6	−51.5	48.7	−8.3	50.7
200	−34.3	55.9	−25.7	58.4	−61.7	54.6	−12.2	55.5
201	−35.3	53.6	−29.3	56.7	−54.5	52.3	−10.2	55.7
202	−15.7	22.1	4.1	34.6	−72.7	−1.8	−21.1	15.0
203	−44.1	15.2	−40.9	19.4	−50.4	17.2	−10.6	25.4
204	−25.9	27.0	−19.6	35.3	−43.2	24.3	−9.2	30.7
205	−33.7	26.7	−23.2	35.8	−54.0	26.3	−12.3	33.6
206	−30.5	26.1	−21.8	35.7	−47.1	27.5	−9.7	34.9
207	−15.9	30.2	5.4	42.8	−80.6	14.1	−19.4	24.1
208	−38.5	30.7	−37.7	30.1	−45.0	31.8	−9.0	34.2
209	−25.1	40.1	−20.0	44.9	−46.4	39.0	−7.5	41.0
210	−32.2	40.8	−23.4	44.9	−55.5	41.0	−11.4	43.3
211	−25.2	43.1	−20.1	46.2	−42.5	45.1	−8.3	45.7
212	−15.1	15.0	4.0	28.2	−70.9	−8.5	−20.1	8.5
213	−40.9	8.6	−37.8	13.5	−46.6	11.3	−8.4	20.2
214	−25.1	26.5	−16.3	36.2	−45.0	25.4	−6.6	30.5
215	−32.5	18.0	−20.5	28.8	−51.7	18.6	−9.9	27.7
216	−30.3	23.1	−21.4	33.0	−45.9	22.8	−9.2	30.3
217	−16.3	21.0	4.5	34.7	−77.6	−1.6	−20.8	14.3
218	−45.2	13.0	−42.2	17.6	−52.0	15.5	−10.7	23.8
219	−27.4	32.9	−19.5	41.9	−49.0	31.4	−9.3	35.2
220	−34.5	27.5	−25.3	36.7	−54.2	26.4	−11.9	34.0

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Table 22 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
221	−35.0	29.0	−25.4	38.5	−50.2	29.0	−9.4	36.8
222	−14.9	36.3	5.4	45.5	−82.9	23.7	−19.8	28.0
223	−44.6	17.0	−42.1	21.3	−52.0	19.0	−10.5	27.9
224	−27.3	41.2	−22.9	44.4	−50.0	40.2	−8.9	41.9
225	−32.9	26.6	−23.7	35.7	−51.0	25.4	−11.5	34.0
226	−33.4	32.5	−24.8	41.7	−52.9	33.9	−10.6	40.8
227	−15.4	12.2	4.8	26.3	−75.3	−10.1	−19.8	5.8
228	−35.9	3.0	−32.5	7.7	−39.8	6.3	−5.9	14.8
229	−25.2	16.7	−18.5	24.9	−42.3	15.2	−7.9	21.0
230	−28.2	11.1	−21.0	18.5	−40.3	10.9	−8.8	18.5
231	−24.9	15.1	−13.9	26.1	−37.9	18.6	−6.1	24.5
232	−15.3	16.2	4.7	29.9	−76.1	−5.7	−19.8	9.9
233	−41.8	11.0	−38.8	15.3	−48.0	13.7	−8.2	21.9
234	−25.2	29.3	−17.5	38.4	−46.9	28.2	−7.6	31.7
235	−34.1	19.8	−25.2	28.7	−52.6	19.6	−9.6	28.7
236	−27.2	21.6	−20.0	30.6	−41.3	20.7	−8.0	27.8
MAXD	−52.5	84.9	−43.3	86.0	−86.5	81.9	−22.8	85.2
MD	−27.4	39.4	−18.6	44.2	−47.3	36.1	−9.3	40.7
MAD	27.4	39.4	20.5	44.2	47.3	36.6	9.4	40.7

Table 23: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the B2PLYP functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−12.3	25.4	−1.5	25.5	−8.6	24.8	22.8	27.7
2	−16.5	25.8	−4.0	26.1	−11.7	26.0	23.7	28.7
3	−14.1	23.7	−3.3	23.8	−10.2	23.5	22.0	26.8
4	−17.0	26.7	−4.3	27.0	−12.3	26.8	24.3	29.6
5	−15.2	25.6	−3.7	25.6	−11.2	25.2	23.5	28.6
6	−17.1	27.0	−4.4	27.3	−12.6	27.1	24.6	30.1

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Table 23 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
7	−15.1	25.7	−3.7	25.7	−11.3	25.3	23.5	28.7
8	10.7	27.0	30.7	35.3	−55.4	8.6	6.6	21.9
9	10.7	28.0	31.3	36.2	−57.6	11.5	7.4	23.6
10	−2.7	8.8	21.7	25.4	−61.8	−8.1	−1.6	10.8
11	−0.8	11.3	22.7	26.5	−61.4	−4.7	−0.1	12.5
12	11.0	27.4	30.9	35.5	−55.6	9.1	7.4	22.7
13	12.2	29.7	32.8	37.8	−56.3	13.0	9.0	25.3
14	−2.5	9.1	21.8	25.6	−61.8	−7.8	−1.4	11.0
15	1.1	15.2	25.0	29.2	−62.2	0.7	2.0	15.9
16	13.1	31.0	33.1	38.1	−55.8	12.6	9.2	25.7
17	12.4	30.0	33.0	38.2	−56.3	13.3	9.2	25.8
18	−2.0	10.1	22.4	26.4	−61.6	−6.9	−0.7	12.1
19	1.8	16.4	25.7	30.0	−62.2	2.2	2.3	16.9
20	13.3	31.4	33.3	38.4	−56.0	12.8	9.4	26.0
21	22.6	41.1	26.8	41.2	20.2	41.1	39.6	42.6
22	5.4	18.7	11.6	23.7	5.6	22.6	25.1	27.4
23	22.1	41.6	26.6	42.2	20.2	41.7	40.4	43.6
24	20.3	39.5	24.9	40.2	18.1	39.7	38.0	41.1
25	21.3	41.3	26.0	41.8	18.8	41.2	39.8	43.0
26	20.9	39.3	25.3	39.8	18.9	39.3	38.1	41.1
27	22.4	40.7	26.4	40.7	19.7	40.5	39.3	42.4
28	23.6	42.2	27.6	42.0	21.2	42.0	40.3	43.4
29	22.5	42.2	27.0	42.7	20.6	42.3	40.8	44.2
30	22.7	44.4	27.9	44.6	20.9	44.2	42.2	45.5
31	12.6	29.1	18.6	32.5	12.1	32.0	33.1	35.8
32	22.5	44.4	27.6	44.7	20.3	44.4	42.3	45.8
33	24.5	43.1	28.3	43.0	21.8	42.5	40.9	44.4
34	24.0	42.6	27.8	42.4	21.4	42.1	40.6	43.8
35	23.8	43.7	28.3	44.2	21.8	43.6	42.2	45.8
36	24.8	47.2	29.9	47.4	22.5	47.1	45.1	48.6
37	25.8	44.4	29.6	44.3	23.2	43.8	42.3	45.7
38	8.0	34.2	13.7	32.0	−15.4	29.2	28.1	34.8

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Table 23 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
39	9.3	36.7	17.0	36.0	−17.0	33.0	30.4	37.8
40	7.9	34.3	13.9	32.4	−15.9	29.3	28.7	35.6
41	9.7	38.7	17.8	38.1	−17.3	35.0	32.1	40.0
42	8.4	34.8	14.2	32.8	−15.9	29.5	29.3	36.2
43	10.5	40.0	18.5	39.2	−17.0	36.0	33.1	41.2
44	8.1	34.6	13.9	32.6	−16.2	29.2	29.1	36.0
45	19.2	43.7	23.9	45.2	4.5	40.0	46.8	51.2
46	−3.0	9.8	0.0	14.7	−13.5	8.3	21.1	24.0
47	8.7	27.7	12.3	27.3	−2.4	23.6	30.1	33.4
48	20.0	48.3	25.8	50.6	4.8	44.9	51.5	56.5
49	−0.9	18.7	4.7	23.7	−10.8	17.5	28.9	32.2
50	8.0	29.1	12.8	29.0	−4.4	25.3	32.0	35.6
51	17.4	41.5	22.6	42.8	3.6	37.9	45.3	49.5
52	21.0	50.8	27.2	53.1	5.9	47.5	53.9	59.2
53	0.6	21.9	6.6	26.6	−9.9	20.9	31.7	35.5
54	8.1	30.2	13.4	30.1	−4.3	26.5	33.1	37.0
55	18.8	43.0	23.9	44.0	5.8	39.0	45.9	50.0
56	−4.8	28.2	8.4	29.1	−8.8	24.7	23.9	28.8
57	−8.3	30.2	7.0	31.5	−11.6	27.1	26.1	31.1
58	−5.2	27.8	7.9	28.6	−9.2	24.3	23.9	28.7
59	−5.0	31.7	7.6	31.1	−10.9	27.1	25.4	30.8
60	−5.3	27.7	7.6	28.4	−9.5	24.0	23.8	28.7
61	−8.2	32.8	7.7	33.9	−11.8	29.6	28.0	33.8
62	−5.4	27.6	7.6	28.4	−9.7	23.9	23.8	28.7
63	14.4	41.7	21.2	40.7	−10.9	39.5	35.8	42.9
64	−28.0	9.6	−13.7	14.2	−20.0	14.7	16.7	20.9
65	−27.6	5.0	−14.3	10.4	−19.1	11.1	13.9	17.4
66	−27.5	10.7	−13.6	15.0	−20.0	15.5	17.0	21.8
67	−25.8	9.7	−13.5	13.8	−18.9	14.4	15.5	19.7
68	−27.0	6.2	−13.9	11.4	−18.9	12.1	14.8	18.5
69	−27.8	11.0	−14.2	15.1	−20.8	15.5	17.3	21.6
70	−26.6	9.5	−14.0	13.5	−19.6	14.2	15.8	19.7

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Table 23 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
71	−27.1	6.2	−14.3	11.4	−19.4	11.9	14.6	18.5
72	−27.3	11.5	−13.9	15.5	−20.5	15.9	17.3	22.3
73	−26.2	9.7	−13.8	13.8	−19.5	14.2	16.1	20.0
74	−27.1	6.4	−14.3	11.5	−19.5	12.0	14.7	18.7
75	−0.3	11.5	25.1	28.7	−64.1	−5.6	1.9	14.1
76	1.6	14.8	26.2	30.2	−62.6	−2.9	3.7	16.5
77	0.9	13.9	24.2	28.1	−61.3	−2.6	2.8	15.0
78	0.3	12.2	25.2	28.9	−63.4	−4.9	2.8	14.7
79	1.9	15.6	26.3	30.7	−62.6	−1.9	3.6	17.3
80	2.1	15.2	25.1	29.2	−59.9	−1.1	3.2	16.5
81	0.3	12.7	25.1	29.1	−63.4	−4.4	2.5	15.1
82	2.5	16.3	26.9	31.3	−61.9	−1.2	4.3	18.1
83	2.1	15.3	25.5	29.7	−60.7	−1.6	3.5	17.0
84	1.1	13.4	25.8	29.7	−62.7	−3.7	3.2	16.0
85	3.0	19.8	9.5	22.6	1.8	22.1	24.0	25.9
86	7.4	23.5	13.6	26.1	6.8	25.8	26.8	29.1
87	6.6	18.6	10.6	20.9	4.4	19.1	25.9	28.1
88	6.7	22.3	13.1	25.0	6.5	24.6	25.5	28.1
89	3.3	20.2	9.6	22.7	1.9	22.2	23.5	25.9
90	7.0	24.1	13.3	26.3	6.9	26.3	26.6	28.8
91	3.3	20.3	9.6	22.7	1.9	22.3	23.6	26.0
92	7.1	24.2	13.5	26.4	7.0	26.4	26.7	29.0
93	7.9	24.0	14.0	26.5	7.1	26.1	27.0	29.5
94	8.0	24.1	14.0	26.5	7.1	26.2	27.3	29.6
95	6.4	23.8	11.8	25.6	4.8	25.3	25.6	28.2
96	7.8	25.0	14.2	27.2	7.8	27.2	27.3	29.7
97	6.2	23.7	11.6	25.6	4.4	25.4	25.7	28.2
98	7.7	20.3	11.2	21.7	5.3	20.4	26.5	28.3
99	8.7	24.7	14.2	26.7	7.5	26.3	27.1	29.3
100	8.7	25.0	14.7	27.4	7.6	27.0	28.3	30.5
101	10.9	25.1	15.5	27.1	9.7	26.3	27.2	29.4
102	7.6	24.7	14.0	27.0	7.3	26.8	27.3	29.6

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Table 23 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
103	7.1	25.1	12.7	26.8	5.6	26.8	26.8	29.1
104	7.7	24.7	14.1	27.1	7.4	26.8	27.3	29.7
105	8.4	23.9	14.6	26.6	7.9	26.0	27.0	29.8
106	8.8	25.0	14.8	27.4	7.8	27.0	28.5	30.4
107	−4.6	17.0	4.6	21.7	−27.8	16.2	19.2	25.6
108	−7.6	8.9	1.2	15.7	−29.5	8.5	14.8	19.5
109	−3.9	19.0	5.3	23.5	−27.6	17.8	20.8	27.1
110	−4.0	18.1	4.4	21.6	−25.8	16.8	18.5	24.7
111	−6.1	11.8	2.4	18.1	−28.9	11.1	16.5	21.8
112	−3.1	20.6	6.2	25.0	−27.3	19.1	21.7	28.3
113	−3.6	18.5	4.8	22.0	−25.5	17.2	19.1	25.2
114	−5.6	13.2	2.9	19.2	−28.7	12.2	17.2	23.0
115	−2.8	20.9	6.5	25.2	−27.1	19.3	22.3	28.6
116	−3.5	18.6	4.8	22.1	−25.7	17.1	19.2	25.3
117	−5.5	13.4	3.0	19.3	−28.7	12.4	17.5	23.1
118	3.2	19.5	7.1	23.3	−8.3	18.3	28.0	31.2
119	4.1	19.1	6.6	19.4	−7.9	15.4	23.1	25.7
120	1.4	16.0	4.6	20.4	−9.5	15.3	26.2	29.1
121	3.1	19.0	6.6	19.7	−8.7	16.1	23.2	26.1
122	5.8	22.6	9.3	26.0	−7.2	21.2	30.5	33.5
123	4.4	21.1	7.1	21.5	−7.3	17.1	24.6	27.6
124	3.3	19.9	6.6	23.1	−10.3	18.7	28.1	31.6
125	5.1	23.1	8.4	23.0	−6.3	19.5	25.6	28.9
126	3.7	20.2	6.8	20.4	−7.8	16.8	23.7	26.7
127	5.4	23.6	9.6	26.8	−7.6	22.2	31.2	34.8
128	−18.0	13.0	−1.6	17.7	−19.2	13.4	16.0	20.3
129	−18.9	9.3	−2.8	14.6	−19.2	10.4	13.5	17.2
130	−16.9	14.0	−1.4	18.2	−18.7	14.1	16.8	21.1
131	−16.9	13.0	−2.4	17.0	−18.5	13.2	15.4	19.5
132	−18.0	10.4	−2.3	15.5	−18.6	11.4	14.5	18.2
133	−17.2	15.0	−1.3	19.2	−19.2	14.9	16.9	21.8
134	−17.0	12.8	−2.5	16.8	−18.6	13.1	15.5	19.3

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Table 23 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
135	−17.7	10.9	−2.4	15.9	−18.8	11.7	14.5	18.6
136	−16.9	15.3	−0.9	19.5	−18.9	15.3	17.6	22.3
137	−16.7	13.2	−2.2	17.2	−18.5	13.4	16.0	19.9
138	−17.5	11.4	−2.1	16.3	−18.7	12.1	14.9	19.0
139	−2.2	17.2	6.4	21.5	−23.9	17.5	20.7	26.1
140	−0.6	20.9	8.1	25.0	−23.1	20.7	23.3	29.1
141	−1.2	18.7	6.6	22.0	−22.0	18.4	20.4	25.4
142	−26.7	−2.5	−17.2	5.3	−28.3	0.5	8.9	13.9
143	−26.2	−4.3	−17.3	3.6	−26.3	0.0	6.9	11.8
144	−25.4	−4.1	−17.0	4.0	−25.6	0.4	7.8	12.4
145	−24.8	−2.2	−14.8	6.1	−25.6	1.2	10.3	14.8
146	−24.4	−3.9	−15.1	4.4	−23.9	0.7	8.5	12.4
147	−24.4	−3.8	−14.8	5.1	−23.6	1.5	9.4	13.6
148	1.0	8.3	22.1	25.0	−49.0	−11.6	−0.6	8.4
149	2.6	16.9	23.6	27.9	−64.3	−10.0	−1.1	12.3
150	−17.9	2.3	−11.4	8.1	−20.5	5.5	11.9	15.9
151	2.7	30.6	2.8	30.5	−5.8	28.8	26.4	32.9
152	0.4	13.2	6.6	19.6	−14.3	12.2	15.3	18.6
153	13.1	30.4	14.5	29.5	−5.8	22.5	24.2	28.7
154	−10.3	3.6	0.6	12.9	−25.3	4.1	10.1	14.3
155	−0.8	16.7	5.5	21.2	−14.6	15.3	18.7	22.6
156	4.6	23.6	11.2	25.6	−16.1	20.1	20.1	25.3
157	1.7	20.7	6.4	22.3	−13.4	17.4	21.5	25.4
158	0.5	7.9	21.6	24.5	−49.4	−11.9	−0.5	8.4
159	0.7	8.2	21.7	24.6	−49.3	−11.8	−0.4	8.4
160	−18.0	2.1	−11.6	7.9	−20.8	5.2	12.0	16.0
161	4.1	32.7	4.3	32.6	−2.5	32.4	28.4	35.0
162	−1.6	9.3	5.1	17.8	−13.3	7.9	14.1	16.9
163	11.5	30.1	15.4	31.4	−7.7	25.4	26.3	30.8
164	−11.5	2.2	−2.3	11.0	−23.3	2.8	9.0	12.8
165	−2.9	8.9	4.7	17.6	−14.3	9.0	14.4	17.2
166	0.8	23.0	9.6	25.3	−21.3	19.8	21.5	27.7

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Table 23 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
167	−1.2	17.5	5.9	22.5	−16.0	14.5	21.0	24.5
168	0.4	7.8	21.6	24.5	−49.7	−12.0	−0.3	8.6
169	0.7	8.4	21.9	24.9	−49.8	−11.6	−0.1	8.9
170	−18.0	2.0	−11.2	8.0	−20.0	5.5	11.4	15.4
171	−12.9	13.8	−9.0	17.3	−19.5	14.4	17.7	23.7
172	2.9	16.0	11.7	25.5	−13.1	15.0	19.1	22.4
173	7.0	27.1	12.0	29.9	−13.2	23.9	24.7	29.9
174	−4.1	7.2	3.4	16.3	−15.3	7.7	13.7	16.4
175	−4.2	19.8	6.2	24.1	−26.2	18.0	20.4	26.8
176	1.7	22.6	10.3	27.2	−16.1	23.3	24.8	30.3
177	0.8	8.2	21.9	24.8	−49.0	−11.6	0.1	9.0
178	7.2	25.1	28.0	33.1	−62.9	4.1	4.3	20.4
179	−17.8	2.2	−11.0	8.1	−19.8	5.6	11.6	15.6
180	−19.0	1.1	−12.7	6.8	−22.0	4.0	11.1	15.1
181	5.4	23.0	13.1	30.1	−13.4	21.0	24.2	28.5
182	6.4	24.8	13.8	31.4	−12.8	22.8	25.5	30.1
183	−10.8	2.7	−1.8	11.5	−22.7	3.1	9.8	13.5
184	−3.8	7.5	3.7	16.5	−14.9	7.9	13.9	16.6
185	−4.5	16.8	5.8	22.9	−25.8	15.8	19.0	25.1
186	−1.3	16.2	7.4	23.5	−17.3	17.9	20.9	25.9
187	2.9	16.5	27.4	31.5	−60.3	−5.4	2.8	16.0
188	−14.6	14.0	−9.2	18.1	−21.8	13.3	19.6	25.4
189	6.7	26.0	15.6	34.5	−13.5	23.1	27.1	31.5
190	−5.4	17.2	6.0	24.5	−28.2	15.0	20.4	26.4
191	−1.4	17.1	7.9	25.6	−19.1	17.0	22.2	27.1
192	4.0	19.7	29.2	34.0	−62.4	−1.0	4.4	19.1
193	−15.7	13.5	−10.7	17.7	−23.3	13.1	19.0	25.2
194	6.8	27.3	15.8	35.9	−14.2	24.3	28.3	32.9
195	−6.4	17.6	6.4	25.3	−30.1	15.4	20.9	27.1
196	−2.1	17.8	8.5	26.8	−20.6	18.2	23.1	28.1
197	4.2	19.8	29.1	33.7	−63.7	4.7	6.1	20.8
198	−13.2	19.9	−10.4	20.5	−21.0	19.6	20.8	27.6

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Table 23 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
199	8.8	30.9	13.6	34.3	−13.0	28.1	30.0	35.0
200	0.8	28.1	9.9	30.6	−24.3	26.3	26.4	33.4
201	0.8	26.9	8.2	30.4	−15.8	25.4	28.7	33.7
202	2.6	14.5	25.7	29.7	−53.0	−7.7	1.4	13.5
203	−18.6	7.6	−12.2	13.3	−23.1	9.6	15.6	20.9
204	1.8	17.2	10.2	26.3	−13.1	15.1	20.3	24.4
205	−8.7	9.3	2.9	18.5	−27.0	8.7	14.8	20.0
206	−5.1	9.6	5.0	19.6	−19.5	10.8	17.1	21.2
207	2.0	15.8	26.6	30.6	−60.9	1.0	3.5	16.6
208	−13.4	16.1	−10.2	16.7	−18.5	17.2	17.3	23.3
209	5.5	23.9	11.9	29.0	−13.5	22.8	24.7	28.9
210	−4.0	18.1	5.2	22.2	−25.4	17.8	19.1	25.1
211	2.0	20.1	8.2	23.6	−13.3	21.8	21.5	26.3
212	1.1	11.3	23.7	27.2	−53.5	−10.6	−0.2	10.3
213	−18.3	5.1	−12.0	11.4	−22.3	7.8	14.4	19.1
214	3.9	20.4	14.4	30.5	−13.4	19.6	23.8	27.8
215	−10.4	5.4	1.9	15.9	−28.2	5.5	13.8	18.3
216	−5.1	10.8	5.7	21.3	−18.3	10.8	17.7	21.0
217	1.8	13.7	26.0	30.0	−58.2	−7.3	1.3	13.0
218	−20.4	6.5	−14.0	12.5	−25.3	8.9	14.6	20.0
219	4.7	23.1	14.9	32.8	−14.0	22.1	25.2	29.5
220	−7.9	11.3	3.1	20.9	−25.3	10.3	16.7	21.7
221	−6.3	13.6	5.0	23.4	−19.4	13.6	21.1	24.7
222	5.2	22.3	29.4	33.9	−60.4	11.2	6.6	21.6
223	−19.8	6.9	−13.8	12.6	−25.2	8.8	15.0	20.5
224	5.9	26.6	11.4	30.2	−14.3	25.5	26.6	31.9
225	−9.6	7.6	1.0	16.8	−25.8	6.2	13.6	18.3
226	−4.4	13.2	5.8	22.9	−21.4	14.6	20.3	25.0
227	0.4	10.9	24.1	27.5	−58.1	−10.0	−0.5	9.9
228	−17.4	2.3	−11.9	7.8	−20.4	5.2	11.6	15.4
229	−1.2	13.8	7.6	22.7	−16.0	12.6	16.9	20.5
230	−12.4	2.0	−4.0	9.5	−23.3	1.6	7.6	11.5

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Table 23 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
231	−5.5	5.9	7.1	17.5	−16.5	9.6	14.5	17.6
232	0.9	11.7	24.5	27.9	−58.5	−8.7	0.0	10.9
233	−18.6	7.2	−12.2	12.8	−23.1	9.7	15.2	20.5
234	4.8	22.4	14.9	32.2	−13.9	21.9	24.4	28.6
235	−11.6	6.8	−1.7	15.6	−28.6	6.2	14.0	18.8
236	−4.9	9.6	4.6	19.3	−16.6	9.1	15.6	18.4
MAXD	−28.0	50.8	33.3	53.1	−64.3	47.5	53.9	59.2
MD	−1.2	19.6	9.4	25.3	−19.4	16.3	19.7	25.5
MAD	9.8	19.8	13.5	25.3	23.5	17.9	19.8	25.5

Table 24: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the B2PLYP-D3 functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−40.3	−2.7	−30.5	−3.5	−37.3	−3.8	−4.9	0.0
2	−47.0	−4.7	−35.1	−5.0	−42.6	−5.0	−6.2	−1.3
3	−41.9	−4.2	−31.9	−4.8	−38.5	−4.8	−5.6	−0.8
4	−48.4	−4.8	−36.5	−5.2	−44.2	−5.1	−6.6	−1.3
5	−45.3	−4.5	−34.7	−5.3	−41.9	−5.4	−6.1	−1.0
6	−49.0	−4.9	−37.2	−5.4	−45.1	−5.4	−6.7	−1.3
7	−45.4	−4.6	−34.9	−5.5	−42.2	−5.6	−6.4	−1.2
8	−11.3	5.0	6.4	11.0	−81.2	−17.1	−20.7	−5.4
9	−12.0	5.4	6.4	11.3	−84.2	−15.1	−20.5	−4.4
10	−19.5	−7.9	4.4	8.0	−80.8	−27.0	−20.6	−8.2
11	−17.6	−5.5	4.7	8.5	−80.9	−24.2	−20.0	−7.3
12	−11.4	5.0	6.1	10.8	−81.9	−17.2	−20.4	−5.1
13	−10.7	6.7	7.5	12.5	−83.2	−13.9	−19.3	−3.0
14	−19.5	−7.9	4.2	8.0	−81.0	−27.1	−20.6	−8.3
15	−17.4	−3.3	5.0	9.2	−83.6	−20.8	−20.2	−6.2

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Table 24 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
16	−10.4	7.6	6.4	11.4	−83.5	−15.1	−20.1	−3.6
17	−10.8	6.8	7.3	12.5	−83.6	−14.0	−19.5	−3.0
18	−19.4	−7.4	4.2	8.3	−81.3	−26.7	−20.4	−7.7
19	−17.5	−2.9	4.7	9.1	−84.6	−20.1	−20.9	−6.4
20	−10.4	7.7	6.3	11.3	−84.0	−15.2	−20.2	−3.6
21	−12.7	5.8	−11.2	3.3	−17.7	3.3	0.6	3.6
22	−19.9	−6.7	−14.8	−2.7	−21.3	−4.4	−1.1	1.2
23	−14.8	4.7	−12.9	2.6	−19.5	2.0	−0.3	3.0
24	−14.8	4.4	−12.7	2.7	−19.6	2.0	−0.6	2.5
25	−15.9	4.1	−13.6	2.1	−21.1	1.3	−0.9	2.3
26	−14.0	4.4	−11.9	2.5	−18.6	1.8	−0.3	2.7
27	−13.2	5.2	−11.8	2.6	−18.4	2.4	0.1	3.1
28	−12.1	6.4	−10.9	3.6	−17.1	3.6	0.7	3.8
29	−14.9	4.7	−13.2	2.5	−19.7	1.9	−0.5	2.9
30	−15.9	5.8	−13.6	3.0	−20.7	2.6	−0.7	2.7
31	−19.8	−3.4	−15.5	−1.6	−22.4	−2.5	−1.1	1.6
32	−17.0	4.9	−14.5	2.5	−22.1	2.0	−1.2	2.3
33	−12.8	5.9	−11.8	2.9	−18.3	2.4	−0.4	3.0
34	−11.9	6.7	−10.8	3.7	−17.1	3.6	0.8	3.9
35	−14.2	5.6	−12.5	3.4	−19.2	2.7	0.3	3.9
36	−15.8	6.5	−13.5	3.9	−21.1	3.5	0.4	3.9
37	−11.7	7.0	−10.7	4.0	−17.2	3.5	0.7	4.1
38	−27.3	−1.1	−21.4	−3.2	−53.5	−8.9	−9.7	−3.1
39	−29.0	−1.6	−21.1	−2.2	−58.8	−8.9	−11.0	−3.6
40	−28.0	−1.6	−21.9	−3.4	−54.8	−9.6	−9.8	−2.9
41	−30.5	−1.5	−22.4	−2.1	−61.4	−9.1	−11.3	−3.4
42	−27.8	−1.4	−22.0	−3.4	−55.2	−9.8	−9.6	−2.7
43	−30.8	−1.3	−22.8	−2.0	−62.1	−9.1	−11.3	−3.3
44	−28.2	−1.6	−22.4	−3.7	−55.6	−10.2	−9.9	−2.9
45	−32.8	−8.3	−29.1	−7.7	−50.5	−15.0	−8.5	−4.1
46	−32.2	−19.4	−29.7	−14.9	−45.2	−23.4	−8.8	−5.9
47	−26.6	−7.6	−22.1	−7.1	−39.5	−13.5	−6.2	−2.9

Continued on next page

Table 24 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
48	−37.9	−9.7	−33.4	−8.6	−56.4	−16.3	−9.9	−5.0
49	−39.3	−19.8	−34.2	−15.3	−51.9	−23.6	−10.1	−6.8
50	−30.3	−9.3	−24.4	−8.2	−44.7	−15.0	−7.0	−3.4
51	−33.0	−8.9	−28.4	−8.3	−49.4	−15.2	−8.2	−4.0
52	−39.8	−10.0	−35.0	−9.1	−58.2	−16.6	−10.7	−5.4
53	−41.4	−20.1	−35.9	−15.9	−54.7	−24.0	−10.9	−7.2
54	−32.1	−9.9	−25.6	−8.9	−46.5	−15.7	−7.7	−3.7
55	−32.2	−7.9	−27.6	−7.5	−47.7	−14.5	−8.1	−4.0
56	−35.7	−2.8	−22.0	−1.3	−41.9	−8.4	−7.4	−2.5
57	−43.0	−4.5	−27.0	−2.6	−48.8	−10.1	−8.8	−3.9
58	−36.3	−3.2	−22.7	−2.0	−42.4	−8.9	−7.7	−2.9
59	−39.5	−2.7	−25.9	−2.5	−47.6	−9.6	−9.2	−3.9
60	−36.4	−3.4	−23.0	−2.2	−42.8	−9.3	−7.8	−3.0
61	−45.6	−4.7	−29.2	−3.0	−51.9	−10.5	−9.8	−4.0
62	−36.5	−3.5	−23.1	−2.3	−43.0	−9.4	−7.8	−2.9
63	−26.0	1.3	−19.7	−0.2	−55.0	−4.5	−8.2	−1.0
64	−56.1	−18.4	−41.4	−13.4	−47.8	−13.1	−8.9	−4.7
65	−52.9	−20.2	−39.3	−14.6	−44.1	−13.9	−9.0	−5.5
66	−56.1	−17.9	−42.0	−13.4	−48.5	−13.1	−9.4	−4.5
67	−51.7	−16.1	−39.5	−12.2	−44.8	−11.5	−8.1	−3.9
68	−52.7	−19.5	−39.4	−14.0	−44.4	−13.4	−8.6	−4.8
69	−57.0	−18.2	−43.4	−14.1	−50.1	−13.8	−9.9	−5.5
70	−52.8	−16.7	−40.4	−12.8	−45.9	−12.2	−8.1	−4.3
71	−53.3	−19.9	−40.4	−14.7	−45.4	−14.2	−9.5	−5.6
72	−56.6	−17.8	−43.1	−13.7	−49.8	−13.4	−9.8	−4.8
73	−52.5	−16.6	−40.3	−12.8	−46.0	−12.3	−8.0	−4.2
74	−53.4	−19.9	−40.6	−14.7	−45.7	−14.2	−9.5	−5.5
75	−19.8	−8.0	4.8	8.4	−86.7	−28.2	−20.9	−8.7
76	−19.4	−6.2	4.0	8.1	−86.9	−27.2	−21.0	−8.2
77	−19.3	−6.2	2.8	6.8	−84.7	−25.9	−20.8	−8.5
78	−19.5	−7.6	4.6	8.2	−86.4	−27.9	−20.3	−8.5
79	−19.5	−5.7	3.6	8.1	−87.4	−26.7	−21.6	−7.9

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Table 24 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
80	−18.3	−5.2	3.5	7.5	−83.6	−24.8	−20.8	−7.4
81	−19.8	−7.5	3.9	7.9	−86.9	−27.9	−21.1	−8.5
82	−18.8	−5.0	4.2	8.6	−86.7	−26.0	−21.0	−7.2
83	−18.7	−5.5	3.5	7.7	−84.8	−25.7	−20.8	−7.3
84	−19.0	−6.6	4.6	8.6	−86.1	−27.1	−20.4	−7.7
85	−22.8	−6.0	−17.5	−4.5	−26.0	−5.6	−3.4	−1.5
86	−21.4	−5.4	−16.5	−4.1	−24.1	−5.1	−3.3	−1.0
87	−19.2	−7.1	−16.1	−5.8	−22.5	−7.8	−1.2	0.9
88	−21.0	−5.4	−16.2	−4.2	−23.2	−5.1	−3.6	−1.1
89	−22.9	−6.0	−17.9	−4.8	−26.3	−6.0	−4.4	−2.0
90	−21.6	−4.5	−16.8	−3.8	−23.9	−4.5	−3.6	−1.4
91	−23.0	−6.0	−18.0	−4.8	−26.4	−6.0	−4.4	−2.0
92	−21.4	−4.3	−16.6	−3.6	−23.7	−4.3	−3.4	−1.2
93	−21.4	−5.3	−16.7	−4.1	−24.3	−5.2	−3.6	−1.1
94	−21.3	−5.2	−16.6	−4.1	−24.3	−5.2	−3.3	−1.1
95	−20.7	−3.3	−16.7	−2.9	−24.4	−3.8	−3.0	−0.4
96	−20.8	−3.7	−16.0	−3.0	−23.1	−3.6	−3.0	−0.5
97	−20.7	−3.2	−16.8	−2.8	−24.6	−3.6	−2.8	−0.3
98	−17.8	−5.2	−15.5	−5.1	−21.4	−6.4	−0.4	1.4
99	−19.2	−3.2	−15.1	−2.6	−22.4	−3.7	−2.4	−0.1
100	−20.6	−4.4	−16.1	−3.4	−23.9	−4.5	−2.5	−0.2
101	−17.2	−3.0	−14.3	−2.7	−20.6	−4.0	−2.7	−0.5
102	−21.2	−4.1	−16.3	−3.3	−23.7	−4.2	−3.1	−0.8
103	−20.7	−2.7	−16.7	−2.6	−24.3	−3.2	−2.8	−0.5
104	−21.0	−4.0	−16.2	−3.2	−23.5	−4.2	−3.1	−0.7
105	−20.3	−4.8	−15.8	−3.7	−23.0	−4.9	−3.3	−0.6
106	−20.6	−4.4	−16.0	−3.4	−23.8	−4.6	−2.2	−0.3
107	−36.1	−14.6	−25.8	−8.8	−62.1	−18.1	−12.8	−6.4
108	−33.8	−17.3	−23.8	−9.3	−58.2	−20.2	−11.3	−6.5
109	−37.0	−14.1	−26.9	−8.7	−63.7	−18.3	−12.9	−6.6
110	−33.8	−11.7	−24.8	−7.6	−58.5	−15.8	−11.9	−5.7
111	−34.2	−16.3	−24.6	−8.9	−59.6	−19.7	−11.9	−6.6

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Table 24 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
112	−37.3	−13.6	−27.2	−8.4	−64.5	−18.1	−13.2	−6.6
113	−33.7	−11.6	−24.7	−7.5	−58.5	−15.8	−11.7	−5.6
114	−34.5	−15.7	−25.0	−8.8	−60.4	−19.4	−12.0	−6.3
115	−37.0	−13.3	−27.0	−8.2	−64.3	−17.9	−12.5	−6.2
116	−34.1	−12.0	−25.3	−8.0	−59.3	−16.5	−12.2	−6.1
117	−34.5	−15.6	−25.1	−8.8	−60.6	−19.5	−12.0	−6.3
118	−34.1	−17.8	−31.1	−14.9	−48.6	−22.0	−10.2	−7.0
119	−26.9	−11.8	−24.1	−11.2	−41.1	−17.8	−7.3	−4.8
120	−33.7	−19.1	−31.2	−15.5	−47.5	−22.7	−9.5	−6.6
121	−28.8	−12.8	−24.8	−11.7	−42.9	−18.1	−8.0	−5.1
122	−32.7	−15.9	−30.3	−13.6	−48.8	−20.4	−9.0	−5.9
123	−28.2	−11.6	−25.3	−10.9	−42.3	−17.9	−7.6	−4.6
124	−34.7	−18.2	−32.3	−15.8	−51.5	−22.4	−10.6	−7.1
125	−28.9	−10.9	−25.5	−10.9	−42.4	−16.5	−8.0	−4.7
126	−28.5	−12.0	−25.0	−11.4	−42.2	−17.6	−8.0	−4.9
127	−35.3	−17.1	−31.9	−14.6	−51.4	−21.7	−10.2	−6.6
128	−46.9	−15.9	−28.9	−9.6	−49.8	−17.2	−11.0	−6.7
129	−45.3	−17.2	−27.7	−10.3	−47.3	−17.7	−11.0	−7.4
130	−45.9	−15.0	−28.9	−9.3	−49.4	−16.6	−10.5	−6.1
131	−43.8	−13.9	−28.2	−8.8	−47.1	−15.4	−9.7	−5.6
132	−44.9	−16.5	−27.7	−9.9	−47.2	−17.2	−10.5	−6.7
133	−47.8	−15.6	−30.5	−10.0	−51.7	−17.5	−12.2	−7.3
134	−44.1	−14.2	−28.5	−9.2	−47.4	−15.7	−9.9	−6.2
135	−45.2	−16.6	−28.5	−10.3	−48.1	−17.7	−11.4	−7.3
136	−47.4	−15.2	−30.0	−9.6	−51.3	−17.1	−11.5	−6.8
137	−44.2	−14.3	−28.7	−9.3	−47.7	−15.9	−10.0	−6.1
138	−45.3	−16.4	−28.6	−10.1	−48.3	−17.5	−11.3	−7.2
139	−31.8	−12.5	−22.2	−7.1	−56.2	−14.8	−9.8	−4.4
140	−33.1	−11.6	−23.7	−6.8	−58.4	−14.6	−10.3	−4.4
141	−30.0	−10.1	−21.7	−6.4	−53.5	−13.1	−9.3	−4.3
142	−50.4	−26.2	−41.5	−19.0	−52.9	−24.1	−12.6	−7.7
143	−47.0	−25.0	−39.0	−18.1	−48.0	−21.6	−11.9	−7.0

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Table 24 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
144	−45.8	−24.6	−38.7	−17.7	−47.0	−21.0	−10.9	−6.3
145	−49.5	−26.9	−40.1	−19.2	−51.2	−24.4	−11.9	−7.4
146	−46.0	−25.5	−37.7	−18.3	−46.6	−21.9	−10.8	−6.8
147	−46.3	−25.7	−37.8	−17.9	−46.4	−21.3	−10.2	−6.0
148	−14.8	−7.4	5.5	8.4	−66.7	−29.3	−18.3	−9.4
149	−16.1	−1.9	2.5	6.8	−85.8	−31.5	−24.4	−10.9
150	−39.8	−19.6	−34.2	−14.7	−43.7	−17.7	−7.3	−3.3
151	−28.7	−0.8	−31.4	−3.7	−39.8	−5.2	−7.1	−0.6
152	−21.2	−8.4	−15.3	−2.3	−38.7	−12.2	−6.0	−2.7
153	−16.1	1.3	−15.5	−0.5	−38.1	−9.7	−6.5	−2.1
154	−29.8	−15.9	−18.2	−5.9	−46.7	−17.2	−9.3	−5.2
155	−26.4	−8.9	−20.4	−4.7	−42.8	−12.9	−7.2	−3.3
156	−21.5	−2.5	−14.9	−0.6	−45.2	−9.0	−7.7	−2.5
157	−26.3	−7.3	−21.8	−5.9	−44.2	−13.5	−7.9	−4.0
158	−15.1	−7.7	5.1	8.0	−67.1	−29.6	−18.1	−9.2
159	−15.0	−7.6	5.1	8.0	−67.1	−29.5	−18.2	−9.3
160	−39.8	−19.7	−34.4	−14.9	−44.0	−18.1	−7.1	−3.1
161	−28.1	0.5	−31.0	−2.8	−37.5	−2.6	−6.1	0.6
162	−23.8	−12.8	−17.2	−4.5	−37.5	−16.3	−6.9	−4.0
163	−19.8	−1.3	−17.1	−1.2	−42.7	−9.6	−7.0	−2.4
164	−31.1	−17.4	−21.4	−8.1	−44.4	−18.3	−10.0	−6.2
165	−25.6	−13.9	−18.2	−5.3	−39.5	−16.2	−8.1	−5.2
166	−28.6	−6.4	−19.4	−3.7	−53.6	−12.4	−9.8	−3.6
167	−30.6	−12.0	−23.4	−6.8	−47.8	−17.4	−8.2	−4.7
168	−15.3	−7.8	5.0	7.9	−67.4	−29.7	−18.0	−9.1
169	−15.1	−7.5	5.1	8.1	−67.7	−29.5	−18.1	−9.1
170	−40.7	−20.7	−35.0	−15.9	−44.1	−18.7	−8.7	−4.7
171	−41.3	−14.6	−39.2	−13.0	−49.9	−16.0	−9.5	−3.6
172	−23.3	−10.2	−15.0	−1.2	−42.5	−14.5	−7.1	−3.7
173	−25.2	−5.1	−20.7	−2.9	−48.9	−11.8	−8.0	−2.8
174	−26.3	−14.9	−18.9	−6.0	−39.9	−16.9	−8.0	−5.3
175	−34.6	−10.6	−23.2	−5.4	−59.2	−15.0	−10.9	−4.4

Continued on next page

Table 24 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
176	−31.6	−10.7	−22.7	−5.8	−52.3	−12.9	−9.5	−3.9
177	−14.8	−7.4	5.4	8.3	−66.6	−29.3	−17.6	−8.6
178	−14.2	3.6	3.6	8.7	−88.2	−21.2	−22.5	−6.3
179	−40.5	−20.5	−34.9	−15.7	−44.0	−18.5	−8.5	−4.5
180	−40.9	−20.8	−35.5	−16.0	−45.3	−19.3	−8.2	−4.1
181	−27.2	−9.6	−20.0	−3.0	−49.4	−15.0	−8.4	−4.1
182	−27.2	−8.8	−20.3	−2.8	−49.9	−14.2	−8.4	−3.8
183	−30.4	−16.8	−20.8	−7.5	−43.6	−17.9	−9.2	−5.5
184	−25.8	−14.6	−18.5	−5.6	−39.3	−16.5	−7.8	−5.1
185	−33.3	−12.0	−22.4	−5.3	−57.2	−15.6	−10.5	−4.4
186	−30.9	−13.4	−21.9	−5.9	−49.6	−14.4	−8.9	−4.0
187	−19.7	−6.2	2.9	7.1	−86.4	−31.4	−23.5	−10.2
188	−46.6	−17.9	−43.4	−16.0	−56.0	−20.9	−10.8	−5.0
189	−30.9	−11.6	−23.1	−4.2	−54.9	−18.3	−10.6	−6.2
190	−39.5	−16.8	−28.1	−9.6	−65.2	−22.0	−14.2	−8.2
191	−35.8	−17.2	−26.9	−9.2	−56.6	−20.6	−12.3	−7.4
192	−20.3	−4.6	3.0	7.7	−90.3	−28.9	−23.8	−9.1
193	−48.4	−19.3	−45.6	−17.2	−58.4	−21.9	−12.1	−6.0
194	−32.8	−12.3	−24.9	−4.8	−58.0	−19.4	−11.3	−6.6
195	−41.9	−17.9	−28.9	−9.9	−68.8	−23.3	−15.1	−8.9
196	−38.3	−18.4	−27.9	−9.6	−60.3	−21.4	−13.2	−8.2
197	−18.7	−3.1	4.1	8.6	−90.7	−22.3	−21.8	−7.1
198	−45.8	−12.7	−44.7	−13.9	−55.8	−15.2	−11.0	−4.3
199	−30.4	−8.3	−26.3	−5.5	−56.0	−14.9	−9.9	−4.9
200	−37.2	−9.9	−27.6	−6.8	−65.5	−14.9	−13.1	−6.2
201	−39.1	−12.9	−31.8	−9.7	−58.9	−17.6	−11.6	−6.6
202	−17.9	−6.0	3.5	7.5	−76.4	−31.1	−22.3	−10.3
203	−47.6	−21.3	−43.2	−17.7	−54.1	−21.4	−11.5	−6.2
204	−29.2	−13.8	−21.7	−5.7	−47.2	−19.0	−10.5	−6.4
205	−36.2	−18.2	−24.5	−8.9	−57.1	−21.5	−13.1	−7.9
206	−33.8	−19.2	−23.8	−9.2	−51.1	−20.7	−11.2	−7.1
207	−18.6	−4.8	4.3	8.3	−84.9	−23.0	−20.9	−7.8

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Table 24 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
208	−41.5	−11.9	−40.0	−13.0	−48.3	−12.7	−9.7	−3.7
209	−28.6	−10.1	−22.6	−5.5	−50.9	−14.6	−9.2	−5.1
210	−34.8	−12.7	−25.1	−8.1	−59.0	−15.8	−12.3	−6.3
211	−28.0	−9.9	−21.9	−6.5	−46.1	−11.0	−9.5	−4.6
212	−17.4	−7.2	3.5	7.0	−74.6	−31.7	−21.3	−10.8
213	−44.2	−20.7	−39.9	−16.5	−50.1	−20.0	−9.2	−4.5
214	−28.7	−12.2	−18.8	−2.7	−49.6	−16.5	−8.2	−4.3
215	−34.8	−19.0	−21.7	−7.7	−54.7	−21.0	−10.4	−5.9
216	−33.6	−17.7	−23.4	−7.8	−49.9	−20.8	−10.4	−7.0
217	−18.7	−6.8	3.9	7.8	−81.5	−30.7	−22.1	−10.4
218	−48.6	−21.7	−44.4	−17.9	−55.6	−21.4	−11.6	−6.1
219	−31.0	−12.6	−21.9	−4.0	−53.6	−17.5	−10.8	−6.4
220	−37.2	−17.9	−26.5	−8.8	−57.5	−21.9	−12.7	−7.7
221	−38.5	−18.7	−27.5	−9.1	−54.5	−21.5	−10.6	−7.0
222	−17.6	−0.4	4.4	8.9	−87.2	−15.6	−21.2	−6.2
223	−47.9	−21.3	−44.2	−17.8	−55.5	−21.5	−11.2	−5.7
224	−30.9	−10.2	−25.7	−6.9	−54.7	−14.8	−10.7	−5.4
225	−35.0	−17.8	−24.5	−8.8	−53.6	−21.6	−11.9	−7.2
226	−36.6	−19.1	−26.6	−9.6	−57.0	−21.1	−12.0	−7.4
227	−17.9	−7.5	4.1	7.5	−79.2	−31.1	−21.3	−10.9
228	−39.3	−19.6	−35.0	−15.3	−43.4	−17.8	−7.2	−3.5
229	−28.5	−13.5	−20.6	−5.5	−46.4	−17.8	−9.5	−5.8
230	−30.1	−15.8	−21.8	−8.3	−42.6	−17.7	−9.4	−5.5
231	−27.7	−16.3	−15.5	−5.1	−41.3	−15.2	−7.2	−4.2
232	−17.7	−7.0	4.1	7.5	−80.0	−30.2	−21.2	−10.3
233	−45.2	−19.4	−40.9	−15.9	−51.5	−18.7	−9.1	−3.8
234	−28.7	−11.1	−19.8	−2.5	−51.3	−15.6	−9.1	−5.0
235	−36.5	−18.1	−26.3	−9.0	−55.6	−20.8	−10.4	−5.5
236	−30.2	−15.7	−21.7	−7.0	−44.8	−19.1	−9.1	−6.4
MAXD	−57.0	−26.9	−45.6	−19.2	−90.7	−31.7	−24.4	−10.9
MD	−30.2	−9.4	−20.3	−4.5	−50.8	−15.1	−10.3	−4.5
MAD	30.2	10.5	21.9	7.9	50.8	15.4	10.3	4.9

Table 25: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the mPW2PLYP functional. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−31.7	13.3	−21.8	13.2	−28.5	13.2	4.2	13.0
2	−37.4	13.1	−25.6	13.3	−33.0	13.8	3.8	13.1
3	−33.4	11.7	−23.4	11.7	−29.9	12.0	3.4	12.3
4	−38.4	13.7	−26.5	13.9	−34.1	14.5	3.9	13.7
5	−35.8	12.9	−25.2	12.8	−32.4	13.1	3.8	13.2
6	−38.7	13.9	−26.9	14.1	−34.7	14.6	4.0	14.1
7	−35.8	13.0	−25.3	12.8	−32.5	13.1	3.6	13.2
8	−5.5	16.8	12.2	23.2	−75.7	−3.0	−25.9	5.3
9	−6.0	17.6	12.3	23.9	−78.6	−0.4	−25.5	6.7
10	−16.7	0.5	6.9	15.9	−78.5	−17.3	−29.1	−1.8
11	−14.6	3.0	7.6	16.8	−78.2	−14.1	−28.1	−0.3
12	−5.5	17.0	12.1	23.3	−76.2	−2.8	−25.4	5.9
13	−4.6	19.3	13.6	25.4	−77.5	1.1	−24.2	8.3
14	−16.5	0.8	6.9	16.0	−78.5	−17.1	−28.9	−1.6
15	−13.5	6.4	8.8	18.8	−80.2	−9.2	−27.4	2.1
16	−3.7	20.7	13.1	25.4	−77.2	0.6	−24.4	8.5
17	−4.6	19.6	13.5	25.7	−77.6	1.3	−25.8	8.6
18	−16.3	1.6	7.1	16.8	−78.5	−16.3	−28.5	−0.6
19	−13.1	7.5	8.9	19.4	−80.7	−7.9	−27.5	2.8
20	−3.5	21.0	13.2	25.6	−77.4	0.8	−24.3	8.7
21	−1.3	22.2	0.2	20.5	−6.3	21.6	12.5	18.6
22	−13.9	3.6	−8.9	7.5	−15.4	7.0	5.1	9.5
23	−2.5	22.2	−0.5	20.8	−7.1	21.4	12.6	19.3
24	−3.1	21.2	−0.9	19.9	−7.8	20.5	11.6	17.9
25	−3.7	21.7	−1.3	20.3	−8.8	20.8	11.9	18.5
26	−2.6	20.8	−0.4	19.4	−7.1	20.0	11.7	17.8
27	−1.8	21.8	−0.3	19.9	−6.9	20.9	12.1	18.4
28	−0.4	23.3	1.0	21.2	−5.2	22.4	13.0	19.4

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Table 25 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
29	−2.3	22.6	−0.5	21.1	−6.9	21.7	12.7	19.6
30	−2.5	24.6	0.0	22.5	−7.1	23.4	13.5	20.3
31	−10.5	11.1	−6.3	13.0	−13.2	13.5	8.5	14.0
32	−3.7	24.0	−1.1	22.1	−8.6	23.0	12.8	20.0
33	0.0	23.9	1.2	21.7	−5.3	22.4	13.0	19.8
34	0.0	23.8	1.2	21.5	−5.1	22.5	13.3	19.7
35	−1.3	23.9	0.5	22.3	−6.1	22.9	13.8	20.9
36	−1.9	26.3	0.5	24.4	−7.1	25.3	15.0	22.3
37	1.3	25.2	2.4	22.9	−4.0	23.6	14.3	21.1
38	−13.2	20.8	−7.3	18.6	−39.6	16.1	4.8	17.0
39	−13.8	21.8	−5.8	21.0	−43.8	18.4	4.8	18.2
40	−13.6	20.8	−7.4	18.8	−40.6	15.9	5.1	17.7
41	−14.5	23.3	−6.2	22.5	−45.5	19.7	5.4	19.5
42	−13.3	21.2	−7.3	19.1	−40.7	16.0	5.5	18.2
43	−14.2	24.2	−6.1	23.2	−45.7	20.4	5.9	20.3
44	−13.6	21.0	−7.7	18.9	−41.1	15.7	5.3	18.0
45	−12.4	20.4	−8.5	21.1	−30.2	16.5	13.0	23.0
46	−22.1	−4.4	−19.7	0.2	−35.4	−6.1	1.5	7.7
47	−13.6	12.4	−9.2	12.3	−26.6	8.4	7.6	15.1
48	−14.9	22.8	−10.1	24.2	−33.5	19.2	14.5	25.7
49	−25.5	1.0	−20.5	5.4	−38.4	−0.5	4.2	11.9
50	−16.0	12.6	−10.2	12.9	−30.7	9.0	8.0	15.9
51	−13.3	19.1	−8.6	19.6	−29.8	15.3	12.7	22.5
52	−15.4	24.4	−10.3	25.7	−33.9	20.9	15.1	27.2
53	−26.1	2.9	−20.6	7.0	−39.6	1.6	5.0	13.2
54	−16.9	13.3	−10.6	13.4	−31.6	9.7	8.2	16.9
55	−12.3	20.3	−7.7	20.5	−27.9	16.1	13.0	22.5
56	−25.1	15.3	−11.4	16.7	−31.3	12.0	3.8	13.3
57	−30.8	16.2	−15.0	18.0	−36.7	13.3	4.0	14.1
58	−25.5	14.9	−12.0	16.1	−31.7	11.5	3.7	13.2
59	−27.5	17.4	−14.1	17.4	−35.7	13.1	3.4	13.7
60	−25.6	14.9	−12.3	15.9	−32.0	11.3	3.6	13.2

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Table 25 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
61	−32.2	17.9	−15.9	19.6	−38.5	15.0	4.3	15.7
62	−25.7	14.8	−12.4	15.9	−32.1	11.2	3.6	13.2
63	−8.8	27.0	−2.4	25.7	−38.0	25.2	9.7	23.0
64	−48.0	−2.8	−33.5	2.0	−39.9	3.1	−0.8	7.0
65	−45.8	−6.4	−32.5	−0.9	−37.2	0.4	−1.9	4.6
66	−47.6	−1.8	−33.8	2.7	−40.2	3.8	−0.8	7.7
67	−44.8	−2.2	−32.9	1.9	−38.1	3.2	−1.2	6.2
68	−45.5	−5.5	−32.4	−0.1	−37.3	1.2	−1.4	5.5
69	−48.2	−1.6	−34.8	2.6	−41.4	3.7	−1.0	7.2
70	−45.7	−2.4	−33.5	1.7	−38.9	3.0	−1.0	6.2
71	−45.8	−5.5	−33.2	−0.2	−38.1	0.9	−2.1	5.2
72	−47.7	−1.1	−34.5	3.1	−41.0	4.1	−0.9	7.9
73	−45.3	−2.1	−33.3	1.9	−38.9	3.0	−0.8	6.5
74	−45.8	−5.3	−33.3	−0.1	−38.3	1.0	−2.0	5.4
75	−15.9	1.1	8.5	17.0	−83.3	−17.3	−28.1	−1.0
76	−14.5	4.2	8.6	18.1	−82.6	−14.8	−27.3	0.8
77	−15.0	3.5	6.9	16.2	−80.8	−14.4	−27.6	−0.3
78	−15.3	2.0	8.5	17.2	−82.7	−16.6	−27.3	−0.4
79	−14.5	5.0	8.5	18.4	−82.8	−14.0	−29.2	1.4
80	−13.9	4.9	7.8	17.2	−79.5	−13.0	−27.4	1.1
81	−15.4	2.3	8.1	17.2	−82.9	−16.2	−27.8	−0.1
82	−13.7	5.7	9.1	19.1	−82.0	−13.2	−27.0	2.2
83	−14.1	4.8	7.9	17.6	−80.6	−13.6	−27.4	1.5
84	−14.6	3.2	8.8	18.0	−82.1	−15.4	−27.1	0.8
85	−15.1	5.8	−9.9	7.2	−18.3	7.4	4.7	8.9
86	−12.3	8.1	−7.5	9.3	−15.1	9.7	6.0	10.6
87	−11.4	4.9	−8.5	5.9	−14.9	5.1	6.8	11.2
88	−12.1	7.5	−7.3	8.9	−14.3	9.2	5.6	10.4
89	−14.8	6.2	−10.0	7.3	−18.3	7.4	4.0	8.8
90	−12.5	9.0	−7.7	9.8	−14.8	10.4	5.8	10.5
91	−14.9	6.2	−10.1	7.4	−18.4	7.5	3.9	8.8
92	−12.3	9.1	−7.6	9.9	−14.6	10.6	6.0	10.7

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Table 25 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
93	−12.0	8.6	−7.4	9.7	−15.0	10.0	6.1	11.0
94	−11.9	8.6	−7.3	9.7	−14.9	10.0	6.3	11.0
95	−12.5	9.3	−8.6	9.7	−16.3	10.2	5.4	10.5
96	−11.6	10.0	−6.9	10.7	−13.9	11.4	6.5	11.5
97	−12.6	9.4	−8.7	9.9	−16.5	10.5	5.7	10.7
98	−9.9	6.9	−7.8	6.8	−13.7	6.6	7.8	11.8
99	−10.3	9.9	−6.3	10.5	−13.5	10.8	6.8	11.5
100	−11.1	9.6	−6.7	10.6	−14.4	10.9	7.3	12.0
101	−7.5	10.7	−4.7	11.2	−10.8	11.1	7.2	11.9
102	−11.9	9.7	−7.1	10.5	−14.4	11.0	6.5	11.4
103	−12.1	10.5	−8.2	10.6	−15.8	11.4	6.1	11.2
104	−11.7	9.7	−7.0	10.6	−14.3	11.0	6.5	11.5
105	−10.5	9.2	−6.1	10.4	−13.2	10.5	6.6	11.9
106	−11.0	9.6	−6.6	10.6	−14.3	10.8	7.6	11.9
107	−24.7	4.2	−14.5	9.3	−51.0	3.6	−1.3	9.8
108	−25.3	−2.6	−15.5	4.8	−50.0	−2.7	−2.8	5.8
109	−24.7	5.9	−14.7	10.7	−51.7	4.8	−0.4	10.9
110	−23.2	6.0	−14.3	9.7	−48.1	4.8	−1.1	9.6
111	−24.5	0.0	−15.1	6.8	−50.3	−0.6	−2.2	7.4
112	−24.3	7.3	−14.3	12.0	−51.8	5.9	−0.1	11.8
113	−22.9	6.4	−13.9	10.1	−47.9	5.2	−0.7	10.1
114	−24.3	1.2	−15.1	7.6	−50.6	0.4	−1.9	8.3
115	−23.9	7.6	−14.0	12.2	−51.6	6.2	0.7	12.1
116	−22.9	6.4	−14.2	10.0	−48.3	4.9	−0.9	10.0
117	−24.3	1.4	−15.0	7.7	−50.6	0.5	−1.7	8.5
118	−20.0	2.4	−17.1	5.4	−34.7	0.8	4.4	11.4
119	−15.2	5.7	−12.6	6.1	−29.6	1.9	4.6	10.4
120	−21.1	−0.6	−18.6	3.1	−35.0	−1.8	3.5	10.1
121	−16.9	5.3	−13.1	6.0	−31.2	2.2	4.2	10.2
122	−17.9	5.2	−15.5	7.7	−34.2	3.3	6.3	13.3
123	−16.1	6.8	−13.5	7.2	−30.5	2.6	4.8	11.2
124	−20.2	2.7	−17.9	5.2	−37.2	1.1	4.3	11.8

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Table 25 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
125	−16.3	8.4	−13.1	8.1	−30.1	4.7	5.0	11.8
126	−16.5	6.3	−13.2	6.4	−30.5	2.7	4.3	10.7
127	−19.7	5.3	−16.3	7.8	−36.0	3.5	5.9	13.6
128	−37.7	0.6	−20.0	6.0	−40.8	1.2	−1.6	6.4
129	−37.1	−2.1	−19.8	3.9	−39.3	−0.9	−2.7	4.3
130	−36.7	1.5	−20.0	6.4	−40.4	1.8	−1.1	7.1
131	−35.8	1.1	−20.4	5.6	−39.2	1.5	−1.5	6.2
132	−36.4	−1.1	−19.5	4.6	−38.9	−0.1	−1.9	5.2
133	−37.6	2.2	−20.6	7.0	−41.7	2.4	−1.9	7.2
134	−35.9	1.0	−20.5	5.5	−39.3	1.5	−1.5	6.0
135	−36.3	−0.7	−19.9	4.9	−39.4	0.1	−2.4	5.3
136	−37.2	2.6	−20.2	7.4	−41.3	2.8	−1.1	7.8
137	−35.7	1.3	−20.4	5.8	−39.4	1.6	−1.3	6.3
138	−36.2	−0.3	−19.8	5.2	−39.4	0.5	−2.2	5.6
139	−20.4	5.8	−10.9	10.6	−45.1	6.6	1.9	11.8
140	−20.0	8.9	−10.7	13.3	−45.6	9.0	3.1	13.9
141	−19.0	7.8	−10.8	11.3	−42.7	7.8	2.0	11.5
142	−44.4	−13.2	−35.7	−5.8	−47.1	−10.1	−6.8	1.7
143	−42.0	−13.9	−34.3	−6.4	−43.2	−9.3	−7.0	1.0
144	−40.8	−13.7	−33.8	−5.9	−42.2	−8.9	−5.9	1.8
145	−43.3	−14.0	−34.2	−6.2	−45.3	−10.4	−5.9	1.9
146	−41.0	−14.5	−32.9	−6.8	−41.7	−9.8	−5.8	1.0
147	−41.0	−14.5	−32.6	−6.1	−41.3	−9.1	−5.0	2.2
148	−13.5	−2.0	6.6	13.6	−65.6	−23.2	−28.2	−5.3
149	−12.1	8.4	6.5	17.6	−82.1	−19.3	−31.4	−2.2
150	−36.5	−10.0	−31.1	−4.4	−40.6	−6.6	−4.4	2.9
151	−19.5	15.0	−22.1	14.0	−30.5	13.0	2.6	14.0
152	−15.0	2.6	−9.2	8.9	−32.7	1.1	0.1	6.2
153	−6.5	16.6	−5.9	15.3	−28.5	8.4	3.5	11.6
154	−24.3	−5.4	−12.8	4.8	−41.4	−4.6	−3.8	3.7
155	−17.7	5.4	−11.7	10.0	−34.3	3.9	1.7	9.0
156	−11.6	13.4	−4.9	15.5	−35.3	9.9	2.5	11.9

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Table 25 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
157	−16.6	8.3	−12.0	9.8	−34.6	4.5	2.3	10.2
158	−13.8	−2.3	6.2	13.2	−66.0	−23.5	−28.0	−5.2
159	−13.7	−2.2	6.2	13.2	−66.0	−23.4	−28.0	−5.2
160	−36.5	−10.1	−31.3	−4.6	−40.9	−6.9	−4.2	3.1
161	−18.6	16.6	−21.5	15.5	−28.0	16.0	3.9	15.5
162	−18.7	−3.2	−12.3	5.4	−32.6	−5.2	−1.9	3.5
163	−8.6	16.2	−5.8	16.9	−31.5	10.6	4.7	13.5
164	−26.4	−7.7	−16.8	2.0	−39.9	−6.8	−5.4	1.6
165	−19.6	−3.5	−12.2	5.5	−33.6	−3.9	−2.2	3.5
166	−17.8	11.3	−8.5	13.8	−43.0	8.3	1.3	12.5
167	−21.0	3.8	−13.9	9.0	−38.5	0.6	1.6	8.8
168	−13.9	−2.4	6.1	13.2	−66.3	−23.6	−27.9	−5.0
169	−13.6	−1.9	6.4	13.5	−66.5	−23.2	−27.8	−4.8
170	−37.2	−11.1	−31.7	−5.5	−40.8	−7.5	−5.6	1.6
171	−35.3	−1.2	−33.4	1.7	−44.0	−0.6	−3.6	6.8
172	−15.5	2.6	−7.3	12.1	−34.8	0.7	0.8	7.3
173	−14.3	13.1	−9.8	15.6	−38.0	9.6	3.3	12.7
174	−20.5	−4.8	−13.2	4.6	−34.3	−4.8	−2.3	3.1
175	−24.2	7.3	−12.9	12.1	−49.1	5.8	−0.2	11.1
176	−19.9	8.0	−11.0	12.5	−40.8	8.6	2.5	12.8
177	−13.5	−2.0	6.5	13.5	−65.6	−23.2	−29.0	−4.5
178	−8.8	15.8	9.1	21.6	−83.0	−6.6	−29.5	4.5
179	−37.0	−10.9	−31.6	−5.3	−40.6	−7.3	−5.4	1.8
180	−37.5	−11.1	−32.3	−5.7	−42.0	−8.0	−5.2	2.2
181	−16.9	7.2	−9.8	14.3	−39.3	4.6	2.0	10.3
182	−16.4	8.8	−9.6	15.2	−39.2	6.2	2.6	11.3
183	−25.7	−7.1	−16.2	2.5	−39.2	−6.6	−4.6	2.2
184	−20.0	−4.5	−12.8	4.9	−33.7	−4.5	−2.1	3.4
185	−23.6	4.9	−12.6	11.5	−47.7	4.1	−0.6	10.1
186	−21.1	2.6	−12.2	10.1	−40.0	4.2	1.1	10.2
187	−15.4	3.8	7.1	17.0	−82.4	−20.0	−30.2	−1.6
188	−39.1	−2.3	−36.0	0.6	−48.6	−3.3	−3.4	7.1

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Table 25 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
189	−18.8	7.6	−11.1	15.6	−43.0	3.8	1.6	10.4
190	−27.5	2.8	−16.1	10.2	−53.5	0.6	−2.1	9.1
191	−24.0	1.2	−15.2	9.3	−45.1	0.6	−0.4	9.1
192	−15.1	6.7	8.0	18.9	−85.6	−15.9	−29.8	0.8
193	−40.7	−3.1	−38.1	0.0	−50.9	−3.7	−4.6	6.5
194	−19.9	8.2	−12.1	16.3	−45.3	4.3	1.8	11.0
195	−29.2	2.8	−16.2	10.7	−56.4	0.6	−2.3	9.2
196	−25.6	1.3	−15.4	10.1	−47.8	1.4	−0.5	9.4
197	−12.6	8.9	10.1	20.7	−85.1	−7.9	−26.7	3.9
198	−36.8	5.5	−35.9	4.8	−46.9	4.8	−1.9	9.9
199	−16.6	13.6	−12.5	16.6	−42.4	10.3	4.2	14.0
200	−22.2	13.7	−12.6	16.2	−50.9	12.0	2.1	14.8
201	−24.6	9.9	−17.4	13.0	−44.6	8.1	3.4	13.2
202	−14.6	2.5	6.6	15.8	−73.3	−21.6	−30.1	−3.1
203	−41.3	−7.5	−37.1	−3.0	−48.0	−5.8	−5.5	4.1
204	−20.2	1.1	−12.9	9.7	−38.4	−2.0	−1.5	6.3
205	−27.1	−2.9	−15.4	6.6	−48.3	−3.7	−3.9	5.4
206	−24.6	−4.6	−14.8	5.5	−42.1	−3.6	−2.1	5.7
207	−14.1	5.5	8.7	18.4	−80.8	−10.8	−27.4	1.0
208	−34.0	3.6	−32.7	3.0	−41.0	4.4	−2.3	8.0
209	−17.1	8.5	−11.2	13.3	−39.6	6.9	2.4	10.7
210	−23.6	6.0	−13.8	10.3	−48.0	5.8	−0.9	9.9
211	−16.5	7.6	−10.6	10.7	−34.8	9.1	2.2	11.2
212	−15.0	0.0	5.7	14.2	−72.4	−23.6	−30.0	−5.0
213	−39.2	−8.9	−35.1	−3.6	−45.2	−6.4	−4.4	4.1
214	−18.9	3.7	−9.1	13.7	−40.0	2.1	1.6	9.2
215	−27.6	−6.2	−14.6	5.1	−47.9	−5.9	−3.2	5.0
216	−24.9	−3.7	−14.8	6.8	−41.4	−4.4	−1.6	5.1
217	−15.3	2.0	7.1	16.4	−78.4	−20.7	−29.8	−3.2
218	−42.5	−8.3	−38.6	−3.3	−49.8	−6.1	−5.7	4.0
219	−19.5	5.7	−10.5	14.9	−42.3	3.8	0.9	9.6
220	−27.5	−1.6	−16.8	7.9	−47.9	−3.1	−2.8	6.3

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Table 25 – continued from previous page

N	6–31G**		6–311G**		def2-SVP		def2-TZVP	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
221	−28.7	−2.2	−17.7	7.6	−44.8	−2.7	−0.5	7.0
222	−11.5	11.5	10.4	21.0	−81.6	−1.2	−26.0	4.8
223	−41.8	−7.8	−38.2	−3.1	−49.6	−6.1	−5.3	4.5
224	−18.5	10.0	−13.4	13.1	−42.5	8.5	2.0	11.9
225	−26.9	−3.8	−16.5	5.6	−45.7	−5.4	−3.8	4.9
226	−25.4	−1.6	−15.5	8.0	−45.9	−0.6	−0.7	8.1
227	−15.5	−0.2	6.4	14.8	−77.1	−22.6	−31.5	−5.1
228	−35.4	−10.0	−31.3	−4.9	−39.8	−7.0	−3.7	3.0
229	−21.1	−0.6	−13.3	7.8	−39.1	−2.6	−2.1	4.9
230	−25.8	−6.8	−17.6	1.1	−38.4	−7.1	−5.2	1.6
231	−21.3	−5.8	−9.2	5.8	−35.1	−2.7	−0.9	5.1
232	−15.0	0.8	6.8	15.3	−77.6	−21.2	−31.0	−4.0
233	−39.7	−6.8	−35.6	−2.1	−46.3	−4.4	−3.8	5.4
234	−18.1	5.9	−9.2	15.3	−40.8	4.5	1.6	9.8
235	−29.1	−4.5	−18.9	4.8	−48.5	−5.0	−2.9	5.7
236	−22.9	−3.5	−14.4	6.0	−37.6	−4.9	−1.7	4.0
MAXD	−48.2	27.0	−38.6	25.7	−85.6	25.3	−31.5	27.2
MD	−21.2	6.0	−11.4	11.0	−41.9	2.3	−3.0	8.7
MAD	21.2	8.8	14.4	11.7	41.9	9.1	8.5	9.3

Table 26: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the LC-BOP functional. All values are without a counter poise correction. MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
1	−45.0	−34.8	−6.3	−43.4	−7.7
2	−51.6	−39.6	−7.7	−49.1	−9.2
3	−46.9	−36.5	−6.9	−45.1	−8.3
4	−53.3	−41.1	−7.9	−50.9	−9.5
5	−50.1	−39.1	−7.3	−48.4	−9.0
6	−54.4	−42.3	−8.4	−52.3	−10.1
7	−50.5	−39.7	−7.6	−49.0	−9.3

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Table 26 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
8	−8.1	−5.0	7.3	−71.9	−14.3
9	−9.6	−6.6	7.0	−75.6	−15.0
10	−18.5	−11.5	2.9	−76.5	−18.7
11	−17.0	−11.1	3.6	−76.1	−18.0
12	−8.5	−5.4	7.3	−72.8	−14.3
13	−8.6	−5.8	8.1	−75.0	−14.1
14	−18.7	−11.7	2.7	−76.9	−18.9
15	−17.1	−11.3	4.1	−78.7	−18.1
16	−8.1	−5.5	8.2	−74.4	−14.4
17	−9.1	−6.5	7.7	−75.7	−14.6
18	−18.9	−12.0	2.6	−77.3	−19.2
19	−17.3	−11.6	3.9	−79.6	−18.5
20	−8.3	−5.8	8.1	−75.1	−14.6
21	−14.5	−11.5	2.3	−18.2	1.2
22	−17.7	−10.6	4.2	−19.0	3.4
23	−17.7	−14.2	0.6	−20.7	−0.8
24	−17.4	−13.7	0.5	−20.8	−0.8
25	−16.4	−12.6	2.4	−20.3	0.9
26	−15.6	−12.2	1.4	−18.9	0.1
27	−15.1	−12.2	2.0	−19.0	0.7
28	−14.4	−11.7	2.0	−17.9	0.8
29	−17.9	−14.5	0.4	−21.0	−1.1
30	−19.5	−15.8	−0.8	−22.7	−2.1
31	−18.5	−12.6	3.6	−20.5	2.0
32	−18.4	−14.6	1.4	−22.1	−0.2
33	−16.1	−13.6	−0.1	−19.9	−1.3
34	−14.5	−12.0	1.8	−18.2	0.5
35	−17.4	−14.0	1.1	−20.7	−0.5
36	−17.5	−13.7	2.5	−21.3	0.9
37	−15.2	−12.8	0.8	−19.0	−0.4
38	−30.5	−29.5	−5.2	−55.5	−9.2
39	−31.3	−28.7	−4.7	−59.4	−9.0
40	−31.6	−30.3	−5.5	−57.2	−9.6

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Table 26 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
41	−33.1	−30.3	−4.6	−62.3	−9.1
42	−31.9	−30.8	−5.7	−58.1	−9.8
43	−33.4	−30.8	−4.7	−63.1	−9.2
44	−32.5	−31.4	−6.1	−58.7	−10.2
45	−34.7	−33.7	−6.4	−51.3	−6.2
46	−33.1	−32.5	−4.7	−46.9	−5.9
47	−28.8	−27.5	−5.4	−42.0	−5.1
48	−40.6	−38.9	−8.7	−57.8	−8.2
49	−40.4	−37.7	−6.7	−53.3	−7.7
50	−32.7	−30.1	−6.3	−47.6	−6.0
51	−36.2	−34.7	−6.8	−52.2	−6.6
52	−42.4	−40.4	−9.1	−59.5	−8.5
53	−42.4	−39.4	−7.0	−56.0	−8.1
54	−34.7	−31.5	−6.8	−49.5	−6.6
55	−35.3	−33.4	−6.7	−50.3	−6.3
56	−39.7	−28.0	−7.5	−46.5	−8.2
57	−47.1	−33.6	−9.6	−53.8	−10.0
58	−40.9	−29.2	−8.4	−47.7	−9.1
59	−43.7	−32.7	−9.7	−53.2	−10.4
60	−41.3	−29.9	−8.8	−48.4	−9.5
61	−50.1	−36.3	−10.3	−57.4	−10.9
62	−41.5	−30.0	−8.9	−48.6	−9.6
63	−29.2	−27.6	−4.2	−56.4	−7.1
64	−58.7	−42.8	−6.2	−52.2	−8.1
65	−55.1	−39.9	−6.4	−47.7	−8.1
66	−59.3	−44.0	−6.8	−53.5	−8.8
67	−55.2	−41.7	−6.9	−50.1	−8.9
68	−55.7	−40.7	−6.6	−48.8	−8.2
69	−60.2	−45.5	−7.7	−55.1	−9.9
70	−56.5	−42.7	−7.5	−51.5	−9.4
71	−56.4	−42.0	−7.5	−50.1	−9.2
72	−60.1	−45.5	−7.6	−55.1	−9.8
73	−56.5	−43.0	−7.8	−51.8	−9.7

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Table 26 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
74	−56.9	−42.4	−7.8	−50.6	−9.5
75	−17.2	−10.2	5.1	−80.1	−16.1
76	−17.1	−11.2	4.4	−80.1	−16.9
77	−17.1	−11.7	3.7	−78.0	−17.2
78	−17.3	−10.7	4.8	−80.1	−16.3
79	−17.7	−12.0	4.0	−80.8	−17.7
80	−16.5	−11.1	4.2	−77.2	−16.7
81	−17.9	−11.5	4.2	−80.7	−17.1
82	−17.2	−11.6	4.4	−80.3	−17.2
83	−17.0	−11.5	4.2	−78.6	−16.8
84	−17.3	−11.0	4.8	−80.1	−16.5
85	−22.4	−15.9	0.8	−25.0	−1.5
86	−19.9	−13.9	1.6	−21.9	−0.6
87	−19.6	−15.9	2.7	−22.5	0.1
88	−20.5	−14.4	0.4	−21.9	−1.6
89	−22.5	−16.4	0.1	−25.4	−2.2
90	−20.7	−14.7	0.2	−22.0	−1.9
91	−22.5	−16.4	0.2	−25.4	−2.1
92	−20.5	−14.5	0.3	−21.9	−1.8
93	−20.1	−14.3	1.3	−22.3	−0.9
94	−20.1	−14.2	1.3	−22.3	−0.9
95	−20.7	−15.9	0.5	−23.7	−1.9
96	−20.2	−14.1	0.8	−21.5	−1.4
97	−20.9	−16.1	0.6	−24.0	−2.0
98	−19.0	−16.0	2.0	−22.2	−0.8
99	−19.4	−14.3	0.6	−21.9	−1.6
100	−19.8	−14.2	1.6	−22.3	−0.7
101	−17.0	−12.9	0.4	−19.2	−1.7
102	−20.6	−14.5	0.5	−22.1	−1.6
103	−20.7	−15.9	0.6	−23.6	−2.0
104	−20.5	−14.4	0.6	−22.1	−1.6
105	−20.6	−14.9	−0.1	−22.5	−2.3
106	−20.0	−14.3	1.4	−22.4	−0.9

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Table 26 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
107	−36.5	−31.1	−4.9	−62.1	−9.7
108	−34.9	−29.0	−5.0	−59.5	−9.2
109	−37.3	−32.0	−5.3	−63.5	−10.2
110	−35.0	−30.6	−5.6	−59.0	−10.4
111	−34.9	−29.5	−5.2	−60.3	−9.5
112	−37.6	−32.5	−5.6	−64.3	−10.7
113	−35.2	−30.7	−5.8	−59.3	−10.5
114	−35.5	−30.4	−5.4	−61.3	−9.9
115	−37.5	−32.5	−5.5	−64.2	−10.6
116	−35.8	−31.4	−6.4	−60.2	−11.2
117	−35.7	−30.7	−5.6	−61.6	−10.1
118	−34.4	−33.4	−6.3	−48.3	−7.9
119	−27.4	−26.8	−5.5	−41.8	−6.1
120	−34.8	−34.4	−6.6	−48.3	−8.2
121	−29.5	−27.8	−5.7	−43.8	−6.6
122	−33.2	−32.9	−6.2	−48.7	−7.8
123	−29.8	−29.2	−6.9	−44.4	−7.3
124	−35.4	−35.2	−7.1	−51.8	−8.9
125	−30.3	−29.5	−6.8	−44.0	−7.8
126	−29.8	−28.6	−6.5	−43.8	−7.2
127	−36.0	−34.9	−6.9	−51.6	−8.5
128	−49.2	−32.5	−8.4	−53.5	−9.7
129	−47.2	−30.6	−8.7	−50.3	−9.8
130	−48.7	−32.9	−8.4	−53.6	−9.9
131	−46.7	−32.0	−8.4	−51.3	−9.8
132	−47.2	−31.0	−8.7	−50.8	−9.7
133	−50.3	−34.5	−9.6	−55.6	−11.0
134	−47.1	−32.4	−8.9	−51.7	−10.2
135	−47.6	−32.0	−9.3	−51.7	−10.4
136	−50.2	−34.4	−9.4	−55.5	−10.8
137	−47.5	−32.9	−9.3	−52.3	−10.7
138	−47.7	−32.1	−9.4	−52.0	−10.4
139	−33.5	−28.8	−4.9	−57.7	−8.3

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Table 26 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
140	−34.6	−29.9	−5.3	−59.4	−8.9
141	−32.4	−28.4	−6.0	−55.5	−9.3
142	−52.4	−40.5	−3.4	−54.8	−11.1
143	−49.4	−38.2	−3.2	−50.1	−11.0
144	−48.0	−37.6	−2.8	−49.2	−10.3
145	−50.4	−37.8	−2.7	−52.1	−9.5
146	−47.5	−35.7	−2.4	−47.8	−9.5
147	−47.5	−35.3	−1.9	−47.6	−8.6
148	−11.9	−5.8	5.6	−60.6	−14.1
149	−12.9	−8.9	3.3	−77.5	−18.6
150	−39.0	−29.7	3.0	−43.8	−2.2
151	−28.4	−29.0	−0.3	−38.8	−3.3
152	−20.3	−14.6	−1.0	−37.5	−2.1
153	−15.6	−16.4	−1.6	−36.2	−2.9
154	−32.0	−23.4	−3.5	−49.0	−7.8
155	−28.8	−24.8	−4.1	−44.8	−6.0
156	−23.3	−20.3	−3.7	−45.4	−6.8
157	−27.7	−26.0	−4.0	−45.5	−5.9
158	−12.5	−6.5	5.5	−61.3	−14.3
159	−12.4	−6.4	5.5	−61.2	−14.3
160	−39.3	−30.2	2.9	−44.3	−2.5
161	−26.8	−27.4	1.6	−35.1	−1.6
162	−21.6	−14.6	0.6	−35.7	−1.4
163	−19.2	−17.0	−2.3	−40.4	−3.0
164	−31.4	−23.5	−1.9	−45.2	−6.3
165	−24.9	−18.7	−0.8	−39.1	−3.5
166	−31.8	−27.5	−5.3	−55.8	−9.1
167	−32.0	−26.6	−3.4	−49.2	−5.5
168	−12.9	−6.8	5.4	−61.8	−14.4
169	−12.7	−6.6	5.5	−62.0	−14.3
170	−38.5	−29.0	2.6	−42.6	−2.5
171	−40.0	−34.3	1.1	−48.6	−4.1
172	−20.8	−12.8	−0.1	−39.4	−1.2

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Table 26 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
173	−24.0	−20.6	−2.4	−46.6	−3.6
174	−25.7	−19.4	−1.0	−39.6	−3.6
175	−37.6	−31.6	−5.7	−61.9	−10.1
176	−33.2	−27.0	−3.9	−52.8	−6.3
177	−12.5	−6.4	5.7	−61.1	−14.1
178	−11.7	−8.8	5.3	−79.2	−17.0
179	−38.5	−28.9	2.7	−42.6	−2.5
180	−40.8	−31.7	1.5	−45.9	−3.9
181	−25.0	−18.3	−1.7	−46.8	−2.5
182	−25.1	−18.6	−1.9	−47.2	−2.4
183	−30.9	−23.2	−1.5	−44.8	−5.9
184	−25.3	−19.0	−0.8	−39.1	−3.3
185	−35.9	−29.5	−5.1	−59.6	−9.5
186	−31.9	−24.7	−3.0	−49.8	−5.6
187	−18.2	−11.2	3.5	−79.0	−19.3
188	−44.7	−37.1	1.2	−53.8	−4.7
189	−26.6	−18.7	−0.7	−49.4	−2.5
190	−39.6	−32.3	−5.0	−64.5	−10.5
191	−34.9	−27.5	−2.8	−54.3	−6.6
192	−19.2	−12.2	3.6	−83.0	−19.8
193	−46.6	−39.3	0.2	−56.4	−5.8
194	−28.7	−20.5	−1.8	−52.5	−3.4
195	−42.4	−33.8	−6.5	−68.5	−12.0
196	−37.9	−29.2	−4.7	−58.3	−8.3
197	−15.8	−10.1	6.4	−82.2	−16.0
198	−42.2	−38.7	1.0	−52.2	−4.3
199	−25.4	−22.0	−0.3	−50.1	−1.7
200	−35.3	−31.0	−3.4	−62.9	−8.4
201	−36.8	−32.3	−3.2	−56.1	−5.9
202	−17.5	−11.1	2.5	−70.6	−19.8
203	−46.6	−37.6	0.0	−53.0	−6.2
204	−26.3	−18.3	−1.1	−43.4	−3.6
205	−38.3	−29.8	−5.7	−58.3	−11.2

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Table 26 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
206	−33.9	−25.1	−3.0	−49.8	−6.7
207	−16.3	−9.7	5.1	−78.1	−16.3
208	−38.8	−34.7	0.6	−45.5	−4.5
209	−25.2	−19.6	−2.0	−46.8	−3.0
210	−35.1	−29.3	−5.2	−58.6	−9.6
211	−26.7	−22.6	−2.3	−43.2	−5.2
212	−16.3	−10.1	3.1	−68.8	−18.6
213	−43.1	−34.1	1.7	−48.8	−4.1
214	−24.9	−15.4	0.5	−44.8	−1.2
215	−36.3	−26.9	−3.5	−56.1	−8.1
216	−33.4	−24.8	−3.4	−49.3	−6.2
217	−17.4	−10.3	3.7	−75.4	−18.8
218	−47.5	−38.6	−0.2	−54.4	−6.4
219	−27.2	−18.1	−1.1	−48.6	−2.9
220	−39.0	−30.6	−5.5	−58.6	−10.7
221	−39.3	−30.1	−4.3	−54.9	−7.4
222	−13.9	−8.6	7.5	−77.6	−15.0
223	−47.6	−39.2	−0.6	−54.9	−6.7
224	−26.8	−22.6	−1.0	−49.8	−2.8
225	−37.2	−29.1	−5.2	−55.1	−10.5
226	−37.1	−28.7	−4.0	−56.0	−8.1
227	−15.7	−8.8	4.2	−72.4	−17.4
228	−36.8	−28.7	2.6	−41.0	−2.0
229	−24.7	−16.7	−0.3	−41.6	−2.5
230	−30.7	−23.6	−2.3	−42.8	−7.0
231	−27.5	−16.2	−0.7	−39.8	−3.1
232	−15.7	−9.0	4.5	−73.3	−17.3
233	−44.4	−35.5	1.1	−50.7	−4.2
234	−24.6	−15.5	0.3	−45.9	−1.1
235	−38.8	−31.1	−4.5	−57.6	−9.1
236	−30.1	−22.1	−3.0	−44.1	−5.5
MAXD	−60.2	−45.5	−10.3	−83.0	−19.8
MD	−30.7	−24.1	−1.9	−50.3	−7.8

Continued on next page

Table 26 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
MAD	30.7	24.1	4.2	50.3	7.9

Table 27: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the M06-L functional. All values are without a counter poise correction. MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
1	−37.5	−32.0	−10.0	−33.5	−11.7
2	−43.5	−36.0	−11.5	−37.5	−13.9
3	−37.5	−31.5	−8.8	−32.6	−10.8
4	−45.0	−37.4	−11.8	−38.7	−14.5
5	−41.4	−34.9	−10.4	−36.1	−12.6
6	−46.5	−38.7	−12.6	−40.1	−15.4
7	−41.4	−35.1	−10.4	−36.4	−12.7
8	−18.3	−15.1	−7.5	−73.4	−19.0
9	−20.5	−16.8	−8.4	−75.5	−20.5
10	−22.5	−15.5	−5.5	−69.4	−19.0
11	−22.3	−15.9	−5.5	−69.9	−19.0
12	−18.0	−14.8	−6.7	−73.1	−18.5
13	−18.9	−15.2	−6.4	−73.7	−18.7
14	−22.0	−15.0	−4.9	−68.8	−18.5
15	−23.5	−16.9	−6.0	−72.2	−19.7
16	−17.8	−14.7	−6.0	−74.0	−18.1
17	−18.9	−15.3	−6.3	−73.8	−18.7
18	−21.8	−14.8	−4.5	−68.6	−18.3
19	−24.0	−17.5	−6.4	−72.8	−20.1
20	−18.0	−14.9	−6.0	−74.4	−18.1
21	−13.3	−12.7	−2.1	−14.2	−1.1
22	−14.3	−12.1	0.7	−10.6	−0.3
23	−13.7	−13.6	−1.6	−13.8	−1.2
24	−14.3	−13.9	−2.6	−14.6	−2.1
25	−15.1	−14.6	−2.9	−15.7	−2.6
26	−12.9	−12.4	−1.4	−13.4	−0.9

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Table 27 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
27	−12.8	−12.4	−1.4	−13.9	−0.8
28	−12.1	−11.7	−0.8	−12.9	−0.1
29	−13.5	−13.3	−1.1	−13.5	−1.0
30	−15.7	−15.0	−2.8	−15.9	−2.5
31	−15.9	−13.5	0.0	−12.3	−0.9
32	−16.1	−15.4	−2.8	−16.2	−2.6
33	−11.6	−11.4	−0.1	−12.7	0.4
34	−11.7	−11.3	−0.3	−12.6	0.2
35	−12.3	−12.2	0.3	−12.4	0.3
36	−14.7	−14.0	−1.1	−14.7	−1.1
37	−10.4	−10.2	1.2	−11.5	1.6
38	−20.7	−21.5	−3.5	−38.0	−6.6
39	−24.3	−23.2	−5.7	−43.0	−9.4
40	−20.2	−20.8	−2.4	−37.9	−5.7
41	−26.4	−25.2	−6.4	−45.4	−10.4
42	−20.0	−20.6	−1.9	−38.0	−5.4
43	−26.3	−25.2	−6.1	−45.4	−10.2
44	−20.4	−20.9	−2.0	−38.2	−5.4
45	−22.9	−23.2	−5.2	−33.0	−4.1
46	−18.7	−19.3	−0.7	−23.6	−2.9
47	−16.7	−17.4	−3.6	−23.4	−2.8
48	−29.1	−28.7	−8.3	−38.4	−7.5
49	−25.0	−23.3	−2.5	−28.0	−4.1
50	−19.8	−19.8	−4.9	−26.9	−4.3
51	−22.1	−21.8	−3.3	−30.6	−2.2
52	−30.8	−30.0	−8.7	−39.7	−8.1
53	−25.5	−23.4	−1.5	−28.3	−3.3
54	−19.5	−19.2	−3.8	−26.1	−3.6
55	−20.3	−19.7	−1.9	−28.4	−0.7
56	−27.5	−21.1	−7.4	−31.6	−8.2
57	−34.9	−26.5	−10.6	−37.7	−11.7
58	−28.1	−21.6	−7.6	−31.9	−8.4
59	−29.1	−22.9	−7.9	−34.3	−8.8

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Table 27 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
60	−28.0	−21.6	−7.4	−32.0	−8.2
61	−37.7	−28.8	−11.4	−40.2	−13.0
62	−27.8	−21.2	−7.0	−31.7	−7.8
63	−19.1	−18.3	−2.6	−36.2	−4.9
64	−49.9	−39.7	−11.1	−38.1	−15.7
65	−47.2	−37.3	−10.8	−34.9	−15.3
66	−50.1	−40.1	−10.9	−38.4	−15.7
67	−45.0	−36.7	−9.2	−34.5	−13.7
68	−47.0	−37.2	−10.2	−34.7	−14.9
69	−51.1	−41.5	−11.8	−39.8	−16.8
70	−45.7	−37.2	−9.4	−35.0	−13.8
71	−46.8	−37.5	−10.3	−34.9	−15.3
72	−50.5	−41.0	−11.1	−39.2	−16.1
73	−45.3	−36.9	−9.0	−35.0	−13.4
74	−46.9	−37.6	−10.3	−35.1	−15.2
75	−26.0	−19.2	−8.3	−73.8	−22.6
76	−24.5	−18.5	−7.3	−71.9	−21.5
77	−24.5	−19.0	−8.1	−70.9	−22.1
78	−24.8	−18.2	−7.0	−72.2	−21.3
79	−24.8	−18.9	−7.5	−72.0	−21.9
80	−23.3	−17.8	−6.8	−69.3	−20.8
81	−25.0	−18.4	−7.0	−72.1	−21.4
82	−24.1	−18.1	−6.6	−71.2	−21.0
83	−23.4	−17.8	−6.5	−69.8	−20.6
84	−24.1	−17.5	−6.0	−71.2	−20.4
85	−21.0	−17.7	−4.9	−18.2	−6.6
86	−21.4	−18.1	−6.0	−17.9	−7.6
87	−12.6	−11.1	2.1	−10.7	0.3
88	−20.8	−17.1	−4.9	−16.8	−6.8
89	−19.9	−16.8	−3.8	−17.1	−5.7
90	−20.6	−17.7	−5.1	−16.5	−7.0
91	−19.9	−16.8	−3.9	−17.2	−5.8
92	−20.4	−17.6	−4.9	−16.3	−6.8

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Table 27 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
93	−20.7	−17.5	−5.2	−17.2	−6.9
94	−20.6	−17.4	−5.1	−17.1	−6.8
95	−19.2	−16.9	−3.9	−16.5	−5.7
96	−19.6	−16.6	−3.9	−15.2	−5.8
97	−19.2	−16.8	−3.7	−16.5	−5.5
98	−10.5	−9.7	3.6	−8.8	1.7
99	−18.9	−16.1	−4.3	−15.6	−5.7
100	−19.7	−16.5	−4.0	−16.3	−5.9
101	−16.3	−14.2	−3.4	−13.6	−4.9
102	−19.5	−16.5	−3.6	−15.4	−5.7
103	−19.0	−16.5	−3.5	−16.0	−5.4
104	−19.5	−16.5	−3.6	−15.4	−5.6
105	−18.4	−14.7	−2.2	−14.5	−4.4
106	−19.7	−16.4	−3.9	−16.2	−5.8
107	−28.1	−25.7	−5.4	−42.4	−11.7
108	−25.2	−23.2	−4.4	−39.1	−10.9
109	−29.0	−26.4	−5.5	−43.3	−11.9
110	−26.2	−24.5	−4.8	−39.5	−10.8
111	−25.7	−23.6	−4.3	−39.9	−10.8
112	−30.0	−27.4	−6.1	−44.4	−12.8
113	−25.6	−23.8	−4.0	−38.8	−10.0
114	−25.7	−23.9	−4.0	−40.0	−10.8
115	−29.5	−27.0	−5.7	−43.9	−12.3
116	−25.7	−24.1	−4.1	−39.2	−10.3
117	−25.5	−23.6	−3.6	−39.7	−10.5
118	−24.5	−23.3	−4.9	−29.0	−6.8
119	−17.9	−18.3	−4.9	−23.3	−6.0
120	−24.8	−24.3	−5.4	−28.5	−7.6
121	−19.6	−19.1	−5.0	−25.3	−6.3
122	−24.3	−23.5	−5.1	−29.7	−7.1
123	−18.3	−18.9	−4.6	−23.1	−5.6
124	−23.1	−22.4	−3.5	−28.9	−5.6
125	−19.4	−19.6	−4.8	−24.3	−6.1

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Table 27 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
126	−18.8	−18.5	−4.4	−23.3	−5.6
127	−23.8	−22.5	−3.4	−29.0	−5.3
128	−37.3	−26.2	−9.7	−35.4	−12.5
129	−35.9	−24.3	−9.5	−32.9	−12.4
130	−34.7	−24.4	−7.5	−33.1	−10.6
131	−34.3	−24.8	−8.5	−32.9	−11.0
132	−35.2	−24.0	−8.8	−32.4	−11.7
133	−37.8	−27.1	−10.0	−36.2	−12.9
134	−33.5	−23.9	−7.6	−32.0	−10.3
135	−35.3	−24.3	−9.0	−32.8	−11.9
136	−37.2	−26.3	−8.9	−35.5	−12.0
137	−33.2	−23.7	−7.4	−31.9	−10.0
138	−35.1	−24.2	−8.7	−32.7	−11.6
139	−21.5	−19.3	−2.2	−33.9	−7.3
140	−22.8	−20.2	−2.2	−35.2	−7.5
141	−19.8	−18.0	−1.5	−31.4	−6.2
142	−40.0	−34.8	−3.7	−38.1	−13.0
143	−38.3	−33.7	−3.8	−35.5	−12.8
144	−37.6	−34.5	−4.8	−36.1	−13.0
145	−40.4	−34.5	−4.7	−37.3	−14.1
146	−38.7	−33.6	−5.0	−35.1	−14.1
147	−39.4	−34.8	−5.9	−36.3	−14.5
148	−9.8	−6.7	0.5	−51.9	−12.0
149	−21.5	−18.1	−9.7	−80.2	−21.1
150	−32.4	−29.3	−1.0	−31.2	−7.5
151	−26.0	−29.1	−3.7	−32.3	−6.6
152	−16.8	−14.4	−4.0	−27.4	−6.2
153	−8.5	−11.7	−1.9	−25.1	−1.9
154	−19.6	−16.4	−0.1	−30.6	−5.4
155	−21.9	−20.5	−5.1	−31.6	−7.7
156	−18.3	−17.5	−4.3	−34.7	−7.1
157	−19.9	−19.6	−4.2	−31.0	−5.8
158	−10.0	−6.8	0.9	−51.9	−11.7

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Table 27 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
159	−10.2	−7.1	0.6	−52.3	−12.1
160	−32.2	−29.1	−0.4	−31.0	−7.1
161	−24.5	−27.6	−2.0	−28.7	−4.7
162	−14.5	−12.0	−1.1	−22.1	−4.1
163	−15.5	−15.4	−4.5	−29.8	−5.0
164	−19.4	−16.5	0.5	−27.5	−4.7
165	−17.6	−15.4	−1.9	−24.9	−6.0
166	−22.0	−21.0	−4.1	−39.0	−7.9
167	−22.3	−21.7	−5.1	−33.2	−8.5
168	−10.1	−6.8	1.2	−52.0	−11.5
169	−10.3	−7.1	1.0	−52.8	−11.8
170	−33.1	−29.7	−1.5	−31.3	−8.3
171	−35.8	−35.4	−4.3	−38.6	−11.0
172	−15.5	−12.4	−2.4	−26.5	−5.5
173	−19.1	−18.2	−4.7	−33.2	−6.5
174	−18.3	−16.1	−1.8	−25.2	−6.1
175	−24.5	−22.3	−2.3	−40.3	−7.3
176	−23.8	−21.1	−3.3	−35.2	−7.5
177	−9.6	−6.3	1.7	−51.3	−11.1
178	−22.2	−18.5	−8.8	−80.8	−21.0
179	−33.1	−29.6	−1.3	−31.2	−8.2
180	−33.2	−30.0	−1.1	−32.1	−7.8
181	−18.2	−16.4	−4.1	−30.9	−6.9
182	−18.5	−16.9	−4.4	−31.7	−7.0
183	−18.6	−15.6	1.2	−26.7	−3.9
184	−17.9	−15.7	−1.5	−24.6	−5.8
185	−23.1	−21.1	−1.8	−38.2	−7.3
186	−22.1	−19.6	−2.1	−32.0	−7.3
187	−15.3	−11.7	−2.7	−65.4	−18.0
188	−39.9	−38.5	−5.4	−41.6	−13.6
189	−23.1	−20.1	−6.5	−35.6	−10.9
190	−27.1	−24.7	−3.5	−42.3	−10.8
191	−25.5	−23.1	−3.9	−36.1	−10.7

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Table 27 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
192	−16.9	−12.8	−3.1	−68.6	−18.8
193	−40.7	−39.2	−5.2	−42.0	−13.7
194	−23.7	−20.4	−6.1	−36.8	−10.7
195	−29.8	−26.0	−4.4	−45.4	−12.2
196	−28.3	−24.6	−4.7	−39.0	−12.1
197	−24.6	−18.9	−7.4	−75.1	−21.5
198	−42.8	−42.3	−8.9	−43.3	−15.3
199	−24.1	−22.9	−7.3	−36.5	−9.9
200	−30.7	−28.4	−7.2	−46.1	−13.1
201	−32.2	−30.0	−8.8	−41.2	−12.6
202	−12.7	−9.2	−1.3	−56.9	−16.6
203	−41.0	−38.1	−5.7	−39.4	−14.6
204	−20.8	−17.5	−4.8	−29.4	−9.8
205	−26.1	−22.4	−3.6	−37.5	−11.1
206	−23.7	−20.2	−2.5	−31.4	−10.0
207	−25.2	−19.0	−8.9	−72.2	−22.7
208	−39.4	−38.0	−7.7	−38.0	−14.0
209	−23.2	−20.8	−7.8	−33.8	−10.7
210	−28.5	−26.0	−6.8	−41.5	−12.7
211	−24.2	−21.5	−5.5	−31.8	−9.9
212	−11.2	−8.8	−1.1	−55.9	−15.5
213	−37.2	−35.0	−3.6	−36.7	−11.9
214	−21.8	−17.6	−5.7	−32.7	−10.4
215	−24.9	−21.4	−2.9	−37.3	−10.0
216	−25.7	−22.1	−5.7	−33.9	−11.3
217	−14.4	−10.8	−2.5	−62.0	−17.4
218	−41.2	−38.7	−5.2	−40.8	−14.0
219	−24.9	−20.9	−7.9	−36.4	−12.5
220	−28.2	−24.4	−5.3	−39.1	−12.0
221	−30.2	−25.9	−6.7	−37.5	−12.6
222	−25.5	−19.8	−8.9	−73.0	−22.3
223	−40.0	−37.7	−4.1	−39.9	−12.8
224	−23.2	−21.5	−6.2	−34.2	−9.0

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Table 27 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
225	−24.5	−21.1	−2.2	−35.5	−9.6
226	−27.1	−23.6	−4.3	−36.5	−11.6
227	−12.8	−10.5	−3.1	−60.8	−16.5
228	−33.8	−32.0	−3.8	−33.7	−10.4
229	−20.3	−17.8	−5.4	−30.4	−9.3
230	−18.7	−17.4	−1.0	−27.3	−6.2
231	−22.0	−16.4	−2.8	−28.3	−8.7
232	−13.4	−10.9	−2.9	−61.5	−16.3
233	−39.0	−37.4	−5.6	−39.3	−12.7
234	−23.1	−19.6	−7.3	−35.0	−10.8
235	−27.6	−25.6	−5.3	−39.6	−11.5
236	−23.6	−20.7	−5.8	−30.9	−10.3
MAXD	−51.1	−42.3	−12.6	−80.8	−22.7
MD	−25.1	−21.7	−4.9	−37.0	−10.1
MAD	25.1	21.7	5.0	37.0	10.2

Table 28: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the M05 functional. All values are without a counter poise correction. MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
1	−30.1	−19.1	10.5	−27.0	9.4
2	−36.2	−23.5	9.7	−31.9	8.5
3	−31.0	−20.3	10.2	−27.6	8.9
4	−36.9	−24.2	10.2	−32.7	8.9
5	−33.8	−22.4	10.5	−30.5	9.1
6	−37.8	−25.1	9.9	−33.8	8.5
7	−33.8	−22.5	10.4	−30.7	9.1
8	−8.3	−2.5	11.5	−78.5	−12.7
9	−9.5	−4.3	11.0	−81.5	−13.9
10	−18.3	−10.9	5.4	−80.1	−18.8
11	−16.3	−10.0	6.8	−80.0	−17.4
12	−7.6	−2.2	12.3	−78.2	−12.1

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Table 28 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
13	−7.7	−2.9	12.6	−80.0	−12.3
14	−17.8	−10.6	5.7	−79.8	−18.5
15	−15.2	−8.9	8.7	−81.7	−16.3
16	−5.8	−0.6	14.6	−79.0	−10.5
17	−7.4	−2.8	12.9	−80.0	−12.1
18	−17.3	−10.2	6.3	−79.6	−18.2
19	−14.6	−8.5	9.2	−81.8	−15.9
20	−5.5	−0.5	14.9	−79.1	−10.3
21	1.6	4.4	21.3	−2.8	17.5
22	−11.3	−8.2	10.5	−13.8	6.0
23	1.2	3.6	22.1	−3.0	18.0
24	−0.6	2.0	19.8	−5.1	15.7
25	−0.1	2.7	20.9	−5.0	16.9
26	1.1	3.4	20.6	−3.2	16.9
27	1.8	4.2	21.3	−2.9	17.5
28	3.3	5.7	22.4	−0.9	18.7
29	1.7	4.0	22.6	−2.4	18.5
30	0.3	3.4	22.2	−3.8	18.3
31	−6.3	−3.2	16.8	−9.3	11.9
32	0.5	3.4	22.7	−4.2	18.7
33	4.2	6.3	23.4	−0.3	19.6
34	4.0	6.2	23.0	−0.4	19.2
35	3.0	5.2	24.0	−1.3	19.8
36	2.6	5.4	25.0	−2.2	20.9
37	5.6	7.7	24.8	1.2	21.0
38	−6.5	−3.7	20.5	−31.4	13.8
39	−7.2	−3.2	21.2	−35.6	14.1
40	−6.3	−3.6	21.1	−31.7	14.5
41	−8.0	−4.0	22.0	−37.2	14.5
42	−5.8	−3.3	21.6	−31.7	15.1
43	−7.4	−3.6	22.8	−37.1	15.3
44	−6.0	−3.6	21.5	−31.9	15.0
45	−5.4	−2.0	23.8	−22.4	24.0

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Table 28 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
46	−16.3	−16.2	8.7	−29.6	5.9
47	−8.5	−6.9	14.2	−21.6	14.2
48	−8.1	−4.0	24.7	−25.8	25.2
49	−19.5	−16.8	11.9	−32.0	9.6
50	−11.2	−8.6	14.2	−25.5	14.4
51	−6.6	−3.3	22.7	−22.3	22.9
52	−7.9	−3.5	26.1	−25.3	26.7
53	−19.1	−16.2	13.8	−32.2	11.5
54	−11.6	−8.4	15.1	−25.8	15.2
55	−4.9	−1.5	23.6	−19.6	24.2
56	−22.2	−9.9	10.8	−28.8	10.1
57	−28.7	−14.5	10.1	−34.7	9.7
58	−22.9	−10.9	10.1	−29.5	9.6
59	−25.3	−13.7	9.4	−33.9	9.4
60	−22.8	−11.1	10.1	−29.6	9.6
61	−29.5	−15.0	11.2	−35.9	10.7
62	−22.0	−10.5	10.7	−28.9	10.2
63	−0.9	2.1	25.1	−28.1	20.0
64	−47.7	−34.3	3.6	−40.3	0.9
65	−45.2	−33.2	1.8	−37.2	−0.7
66	−46.9	−34.2	4.2	−40.1	1.4
67	−45.2	−34.1	2.1	−38.9	−0.3
68	−45.0	−33.4	2.1	−37.5	−0.3
69	−47.3	−35.2	3.7	−41.2	1.0
70	−45.8	−34.7	1.8	−39.5	−0.5
71	−44.7	−33.6	2.1	−37.8	−0.3
72	−46.7	−34.7	4.3	−40.6	1.5
73	−45.3	−34.4	2.1	−39.4	−0.1
74	−44.7	−33.7	2.1	−37.9	−0.2
75	−16.8	−11.4	6.8	−83.8	−17.6
76	−15.0	−10.5	8.0	−82.5	−16.7
77	−16.3	−12.0	6.0	−81.6	−18.1
78	−15.9	−10.9	7.4	−82.7	−16.8

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Table 28 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
79	−14.9	−10.6	8.2	−82.7	−16.9
80	−15.0	−10.9	7.0	−80.1	−17.0
81	−15.8	−11.1	7.5	−82.7	−16.9
82	−14.1	−9.9	8.9	−81.9	−16.1
83	−15.1	−11.0	7.3	−80.9	−16.9
84	−14.9	−10.3	8.3	−81.8	−16.0
85	−15.1	−11.4	8.0	−19.7	3.3
86	−11.8	−8.1	10.6	−15.5	5.8
87	−5.3	−4.2	15.1	−9.5	10.6
88	−11.4	−7.7	10.7	−14.4	6.0
89	−14.4	−11.1	8.2	−19.1	3.5
90	−12.4	−9.2	9.4	−15.6	4.8
91	−14.4	−11.1	8.2	−19.1	3.5
92	−12.2	−9.0	9.6	−15.4	4.9
93	−11.2	−7.8	11.0	−15.1	6.3
94	−11.1	−7.7	11.1	−14.9	6.4
95	−12.7	−10.5	9.2	−17.5	4.2
96	−11.3	−8.2	10.4	−14.5	5.8
97	−12.7	−10.5	9.3	−17.6	4.3
98	−3.6	−3.0	15.9	−7.8	11.6
99	−9.8	−7.2	10.9	−13.9	6.3
100	−10.1	−6.9	12.1	−14.2	7.3
101	−5.9	−4.1	12.4	−9.6	7.8
102	−11.4	−8.3	10.5	−14.8	5.9
103	−11.9	−9.6	10.0	−16.5	5.0
104	−11.3	−8.1	10.6	−14.7	6.0
105	−9.0	−5.7	12.6	−12.2	8.0
106	−10.0	−6.9	12.2	−14.1	7.3
107	−20.1	−15.7	11.1	−46.3	2.7
108	−21.8	−18.0	6.4	−46.4	−1.3
109	−19.6	−15.2	12.2	−46.0	3.7
110	−19.5	−15.7	10.3	−43.5	2.2
111	−20.1	−16.5	8.3	−45.6	0.6

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Table 28 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
112	−19.1	−14.8	12.8	−46.0	4.2
113	−18.9	−15.3	10.6	−43.2	2.7
114	−19.7	−16.6	9.0	−45.6	1.0
115	−18.7	−14.6	13.1	−45.7	4.6
116	−19.0	−15.5	10.5	−43.5	2.6
117	−19.4	−16.4	9.2	−45.5	1.3
118	−14.6	−13.9	11.6	−29.1	9.0
119	−10.5	−11.0	9.8	−24.6	8.7
120	−15.8	−16.3	9.7	−29.9	7.0
121	−12.9	−12.5	9.2	−26.8	8.0
122	−11.9	−11.8	13.4	−27.8	10.9
123	−11.2	−11.9	9.7	−25.2	8.9
124	−14.9	−14.7	11.6	−31.1	9.2
125	−12.9	−12.9	9.6	−26.4	8.5
126	−12.5	−12.5	9.2	−26.1	8.3
127	−13.9	−13.0	13.4	−29.5	11.0
128	−37.2	−22.4	2.3	−41.2	0.0
129	−36.4	−22.2	0.6	−39.2	−1.2
130	−35.4	−21.6	3.2	−39.9	1.0
131	−35.7	−23.1	1.2	−39.6	−0.8
132	−35.0	−21.4	1.7	−38.3	−0.2
133	−36.0	−22.1	3.4	−40.6	1.1
134	−35.2	−22.6	1.5	−39.1	−0.3
135	−34.4	−21.3	2.1	−38.2	0.2
136	−35.5	−21.7	3.8	−40.3	1.7
137	−34.8	−22.3	1.8	−38.9	0.1
138	−34.1	−21.1	2.4	−38.0	0.6
139	−15.4	−11.6	11.7	−39.6	5.6
140	−13.7	−10.2	14.1	−38.6	7.7
141	−14.2	−11.2	11.2	−36.9	5.4
142	−37.3	−29.8	9.7	−41.1	−2.6
143	−35.5	−28.3	9.5	−37.1	−2.6
144	−35.3	−28.2	9.7	−36.5	−1.7

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Table 28 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
145	−37.2	−29.5	8.5	−40.7	−3.0
146	−35.5	−28.3	8.1	−37.1	−3.3
147	−36.2	−28.0	9.0	−36.9	−1.8
148	−11.5	−5.0	7.8	−62.9	−13.7
149	−17.3	−9.9	4.1	−87.7	−20.1
150	−30.6	−24.3	11.7	−34.0	0.7
151	−16.6	−17.5	15.9	−26.5	7.8
152	−13.8	−9.4	6.1	−30.8	1.0
153	−3.8	−3.0	11.8	−24.7	8.6
154	−18.8	−10.7	9.8	−34.8	1.6
155	−16.1	−12.2	9.0	−32.0	4.4
156	−7.5	−3.5	14.1	−29.8	8.3
157	−13.7	−11.0	11.1	−30.9	7.4
158	−11.4	−5.2	8.3	−62.9	−13.3
159	−11.5	−5.3	8.1	−63.1	−13.5
160	−30.3	−24.3	12.1	−34.0	1.0
161	−14.3	−15.2	19.2	−22.6	10.9
162	−13.3	−7.8	8.1	−26.7	2.3
163	−4.4	−1.8	14.5	−25.6	10.7
164	−19.3	−12.3	9.1	−32.0	1.1
165	−14.2	−9.3	8.8	−27.6	2.6
166	−13.1	−7.6	15.2	−36.5	8.5
167	−16.9	−12.1	10.8	−33.8	6.0
168	−11.3	−5.1	8.6	−63.0	−12.9
169	−11.2	−5.0	8.8	−63.4	−12.9
170	−30.8	−24.5	10.7	−33.6	−0.2
171	−30.5	−27.4	12.4	−38.2	1.2
172	−11.3	−4.6	10.3	−29.5	4.7
173	−12.1	−8.4	11.2	−34.6	6.8
174	−14.7	−9.9	8.6	−27.9	2.5
175	−19.1	−12.2	14.1	−42.3	6.5
176	−16.0	−9.8	13.3	−35.8	7.9
177	−10.8	−4.7	9.0	−62.3	−12.6

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Table 28 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
178	−13.9	−7.9	8.1	−87.8	−16.8
179	−30.5	−24.3	11.0	−33.4	0.1
180	−31.1	−25.2	11.3	−34.9	0.3
181	−12.6	−6.9	11.3	−33.9	6.2
182	−12.2	−6.6	11.8	−34.0	7.1
183	−18.2	−11.4	10.0	−31.0	2.1
184	−14.1	−9.4	9.1	−27.2	2.9
185	−17.7	−11.1	13.7	−40.4	5.9
186	−16.3	−10.1	11.6	−34.5	5.5
187	−11.9	−6.4	10.2	−79.3	−15.4
188	−31.2	−28.1	14.4	−40.9	2.2
189	−12.9	−7.0	12.9	−36.8	6.0
190	−19.3	−13.0	14.4	−45.1	4.3
191	−17.0	−11.9	12.5	−38.3	4.3
192	−11.5	−5.9	11.7	−82.3	−14.8
193	−32.6	−30.2	13.6	−42.9	1.2
194	−13.6	−7.7	13.1	−38.5	6.4
195	−21.1	−13.7	14.2	−47.7	4.1
196	−19.3	−12.9	11.9	−41.5	3.7
197	−12.5	−7.4	11.8	−83.9	−13.6
198	−31.0	−30.7	13.4	−40.8	3.2
199	−11.8	−9.4	13.8	−36.7	9.0
200	−15.6	−11.2	17.0	−43.4	8.8
201	−19.9	−16.1	13.4	−39.1	8.7
202	−11.7	−7.0	7.9	−71.0	−16.7
203	−34.1	−30.3	11.5	−41.1	−1.1
204	−14.1	−9.3	9.6	−32.4	2.5
205	−19.7	−13.3	11.2	−40.6	1.5
206	−18.8	−13.3	8.8	−36.7	0.9
207	−16.0	−10.5	7.0	−81.5	−17.2
208	−30.5	−29.3	10.4	−37.2	0.9
209	−14.4	−10.5	9.0	−36.1	4.6
210	−19.7	−14.8	10.4	−43.2	2.9

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Table 28 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
211	−13.1	−9.8	11.2	−30.7	6.0
212	−12.3	−7.5	7.1	−69.8	−16.5
213	−32.1	−28.0	12.4	−38.1	0.4
214	−14.4	−7.1	11.3	−35.2	5.0
215	−21.2	−13.4	10.6	−41.5	2.2
216	−19.6	−13.2	9.7	−35.9	2.9
217	−12.5	−7.2	8.5	−75.5	−16.1
218	−35.1	−31.2	12.2	−42.2	−0.4
219	−13.9	−6.9	12.4	−36.1	5.6
220	−19.8	−13.2	12.9	−39.6	3.5
221	−23.1	−16.1	10.6	−39.3	3.9
222	−12.9	−7.7	11.0	−81.7	−14.2
223	−33.9	−30.5	12.9	−41.5	0.4
224	−15.6	−12.8	10.0	−38.8	5.0
225	−18.1	−12.2	12.4	−36.7	3.4
226	−18.3	−12.7	12.1	−38.6	3.9
227	−13.4	−7.7	6.9	−74.3	−16.3
228	−31.6	−27.0	9.1	−35.6	−0.8
229	−17.2	−11.2	7.7	−34.5	1.1
230	−19.2	−13.8	7.5	−31.2	0.1
231	−17.1	−8.3	8.8	−30.4	2.2
232	−12.7	−7.1	8.0	−74.6	−15.4
233	−34.1	−29.4	11.9	−40.1	0.8
234	−13.5	−6.0	12.2	−35.2	6.0
235	−23.9	−16.9	10.3	−42.9	2.3
236	−18.1	−12.3	8.4	−32.1	2.2
MAXD	−47.7	−35.2	26.1	−87.8	26.7
MD	−17.9	−12.4	11.3	−38.4	2.7
MAD	18.2	13.0	11.3	38.4	8.3

Table 29: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the M05-2X functional. All values are without a counter poise correction. MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
1	−34.3	−25.8	−5.0	−32.2	−3.6
2	−39.7	−29.3	−5.7	−36.5	−4.4
3	−35.6	−26.6	−4.8	−33.3	−3.5
4	−40.7	−30.2	−5.5	−37.6	−4.3
5	−37.9	−28.6	−4.9	−35.6	−3.8
6	−41.6	−31.1	−6.0	−38.7	−4.7
7	−38.0	−28.7	−4.9	−35.9	−3.8
8	−13.5	−9.7	1.9	−78.9	−17.9
9	−13.3	−9.4	3.4	−80.8	−16.9
10	−17.1	−8.5	4.6	−76.1	−15.1
11	−16.0	−8.6	5.1	−76.3	−14.8
12	−13.2	−9.5	2.5	−79.2	−17.4
13	−11.9	−8.1	5.1	−79.6	−15.3
14	−16.9	−8.4	4.8	−76.2	−15.0
15	−16.4	−9.1	5.4	−79.2	−15.2
16	−12.6	−9.4	3.7	−80.3	−17.0
17	−11.9	−8.2	5.2	−79.8	−15.4
18	−16.6	−8.2	5.2	−76.2	−14.8
19	−16.5	−9.4	5.3	−80.0	−15.5
20	−12.5	−9.4	3.9	−80.7	−16.9
21	−8.5	−6.3	5.9	−11.5	5.8
22	−12.0	−5.6	6.4	−12.1	6.4
23	−9.7	−7.0	6.2	−12.2	5.6
24	−9.7	−6.7	5.8	−12.5	5.3
25	−9.8	−7.0	6.1	−13.2	5.5
26	−8.8	−6.2	5.8	−11.7	5.4
27	−8.4	−6.3	6.3	−11.7	6.0
28	−8.0	−6.1	6.1	−10.9	5.9
29	−9.4	−6.8	6.6	−12.0	5.9
30	−10.4	−7.4	6.2	−13.0	5.7

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Table 29 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
31	−12.4	−7.2	6.7	−13.3	5.8
32	−10.7	−7.8	6.6	−13.8	5.9
33	−7.7	−6.0	6.2	−11.0	5.9
34	−7.7	−5.9	6.4	−10.7	6.0
35	−8.2	−5.6	8.0	−11.0	7.2
36	−9.1	−6.3	8.3	−12.4	7.6
37	−6.7	−5.0	7.3	−9.9	7.0
38	−21.7	−21.2	−0.8	−44.9	−2.4
39	−22.4	−20.3	−0.8	−48.4	−2.5
40	−22.1	−21.3	−0.5	−46.0	−2.2
41	−23.8	−21.5	−0.5	−50.7	−2.4
42	−21.9	−21.1	−0.1	−46.1	−1.8
43	−23.4	−21.2	0.1	−50.8	−1.8
44	−22.2	−21.5	−0.2	−46.5	−1.9
45	−19.2	−18.6	3.6	−33.6	5.4
46	−15.5	−15.2	7.8	−26.9	7.4
47	−15.3	−14.4	2.3	−26.6	4.5
48	−22.5	−21.1	3.3	−37.2	5.7
49	−21.5	−19.0	6.2	−32.0	6.4
50	−17.4	−15.4	2.5	−30.2	4.8
51	−19.4	−18.1	4.3	−33.1	6.4
52	−23.1	−21.4	4.0	−37.7	6.4
53	−22.0	−19.3	7.1	−33.0	7.3
54	−18.0	−15.4	3.1	−30.6	5.3
55	−17.8	−16.3	5.3	−30.6	7.4
56	−26.9	−16.7	−3.2	−32.2	−1.0
57	−32.7	−20.8	−4.7	−37.8	−2.1
58	−27.7	−17.5	−3.8	−33.0	−1.5
59	−27.9	−18.3	−2.9	−35.4	−0.9
60	−27.7	−17.6	−3.6	−33.2	−1.4
61	−34.1	−21.8	−4.5	−39.6	−1.9
62	−27.5	−17.3	−3.4	−33.0	−1.1
63	−19.0	−17.9	0.8	−43.6	0.3

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Table 29 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
64	−46.1	−31.7	−4.4	−39.1	−3.8
65	−43.3	−29.4	−4.6	−35.4	−4.0
66	−46.1	−32.1	−4.3	−39.6	−3.8
67	−41.8	−29.2	−3.5	−35.7	−3.2
68	−42.9	−29.1	−3.8	−35.4	−3.2
69	−46.4	−33.0	−4.6	−40.6	−4.4
70	−42.8	−30.0	−4.0	−36.8	−3.5
71	−42.6	−29.3	−3.8	−35.6	−3.3
72	−46.1	−32.7	−4.3	−40.4	−3.9
73	−42.2	−29.7	−3.7	−36.5	−3.2
74	−42.7	−29.4	−3.7	−35.8	−3.3
75	−18.0	−9.0	5.3	−81.7	−14.7
76	−17.4	−9.4	5.5	−81.3	−14.6
77	−16.5	−9.4	5.2	−78.3	−14.6
78	−17.4	−8.8	5.9	−81.1	−14.1
79	−17.3	−9.6	5.6	−81.4	−14.8
80	−15.5	−8.5	6.1	−77.2	−13.7
81	−17.4	−9.0	5.8	−81.1	−14.3
82	−16.7	−8.9	6.3	−80.7	−14.2
83	−15.5	−8.4	6.6	−78.1	−13.4
84	−16.7	−8.3	6.7	−80.4	−13.5
85	−16.2	−10.4	4.8	−17.8	3.1
86	−15.1	−9.9	4.1	−16.1	2.3
87	−12.4	−9.0	7.9	−14.0	5.9
88	−15.4	−9.9	3.8	−15.9	1.9
89	−15.6	−10.1	5.1	−17.5	3.3
90	−14.9	−9.7	4.0	−15.4	2.2
91	−15.6	−10.1	5.1	−17.5	3.3
92	−14.8	−9.5	4.2	−15.2	2.4
93	−14.6	−9.5	4.6	−15.8	2.8
94	−14.5	−9.5	4.6	−15.8	2.8
95	−13.5	−9.1	5.7	−15.5	3.9
96	−14.0	−8.7	5.0	−14.5	3.2

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Table 29 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
97	−13.7	−9.4	5.7	−15.8	3.8
98	−11.2	−8.3	8.2	−13.1	5.9
99	−12.5	−8.0	5.7	−14.0	3.8
100	−13.6	−8.7	5.7	−15.1	3.7
101	−10.1	−6.6	5.6	−11.8	3.6
102	−14.0	−8.7	5.2	−14.7	3.3
103	−13.6	−9.2	5.8	−15.4	3.8
104	−14.0	−8.7	5.2	−14.7	3.3
105	−13.4	−8.2	5.6	−14.5	3.5
106	−13.6	−8.7	5.7	−15.1	3.7
107	−26.9	−21.7	−0.5	−49.9	−3.1
108	−23.5	−18.0	0.9	−45.3	−1.3
109	−27.6	−22.3	−0.7	−51.2	−3.3
110	−25.1	−20.8	−0.7	−46.7	−3.4
111	−23.8	−18.6	0.7	−46.6	−1.6
112	−27.7	−22.5	−0.7	−51.9	−3.5
113	−24.7	−20.3	−0.3	−46.4	−3.0
114	−23.5	−18.5	1.5	−46.6	−1.2
115	−27.2	−22.1	−0.2	−51.3	−3.1
116	−24.7	−20.5	−0.2	−46.7	−3.1
117	−23.2	−18.4	1.7	−46.5	−1.0
118	−19.7	−18.3	3.8	−31.5	3.2
119	−14.6	−13.5	2.6	−27.0	3.4
120	−19.0	−18.1	4.6	−30.1	3.8
121	−16.9	−14.8	1.9	−29.1	2.7
122	−18.4	−17.7	4.0	−31.9	3.5
123	−15.0	−13.7	3.0	−27.4	4.0
124	−19.2	−18.6	4.3	−33.2	3.5
125	−15.6	−14.3	2.8	−27.1	3.5
126	−15.9	−14.2	2.5	−27.7	3.2
127	−19.6	−18.2	4.6	−33.0	4.1
128	−35.1	−19.8	−3.8	−37.7	−2.4
129	−33.9	−18.5	−4.3	−35.5	−2.9

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Table 29 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
130	−33.1	−18.6	−2.2	−36.3	−1.1
131	−32.7	−18.9	−3.3	−35.4	−2.2
132	−33.0	−18.0	−3.5	−35.0	−2.0
133	−34.8	−20.2	−3.7	−38.3	−2.4
134	−32.4	−18.6	−3.0	−35.1	−1.9
135	−32.5	−17.9	−3.4	−34.9	−1.9
136	−34.2	−19.6	−3.2	−37.7	−1.8
137	−32.0	−18.3	−2.7	−35.0	−1.6
138	−32.4	−17.9	−3.2	−34.9	−1.7
139	−22.9	−18.6	0.5	−44.2	−1.0
140	−23.2	−18.7	1.0	−45.3	−0.7
141	−21.2	−17.5	0.3	−41.5	−1.4
142	−39.6	−28.8	2.2	−40.8	−3.8
143	−38.6	−28.4	0.8	−38.2	−5.5
144	−37.7	−28.4	0.2	−38.0	−5.7
145	−37.1	−25.5	3.5	−37.2	−1.8
146	−36.0	−25.1	2.3	−34.9	−3.4
147	−36.4	−25.5	1.7	−35.4	−3.7
148	−11.7	−4.3	5.9	−62.1	−12.3
149	−20.1	−15.3	−3.9	−86.8	−23.7
150	−29.9	−21.7	4.9	−33.6	1.6
151	−22.2	−22.7	1.5	−31.8	1.3
152	−10.7	−5.2	3.8	−26.5	4.5
153	−7.2	−8.3	3.3	−26.5	3.6
154	−22.3	−15.1	0.4	−38.0	−2.2
155	−18.3	−14.6	0.5	−32.5	0.6
156	−17.9	−15.4	−2.6	−38.7	−3.6
157	−18.5	−17.0	−0.3	−34.9	−0.2
158	−12.1	−4.8	6.0	−62.5	−12.3
159	−12.0	−4.8	5.9	−62.5	−12.4
160	−29.9	−21.8	5.2	−33.7	1.8
161	−22.1	−22.8	1.6	−29.3	1.1
162	−12.2	−6.0	5.0	−25.0	4.5

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Table 29 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
163	−12.1	−10.0	0.9	−32.4	2.2
164	−23.3	−16.3	0.9	−35.8	−1.9
165	−14.6	−9.1	3.5	−27.3	2.2
166	−23.6	−20.0	−2.2	−45.7	−3.8
167	−19.2	−15.3	1.7	−34.7	1.5
168	−12.2	−4.8	6.2	−62.7	−12.2
169	−12.1	−4.8	6.2	−63.0	−12.1
170	−30.3	−21.8	4.1	−33.3	0.7
171	−28.9	−24.2	5.2	−36.4	2.0
172	−10.4	−3.2	4.8	−27.8	5.5
173	−14.6	−11.2	2.4	−35.6	3.1
174	−15.4	−9.8	3.3	−27.7	2.1
175	−25.7	−21.0	0.3	−48.1	−2.2
176	−21.1	−16.0	1.8	−38.6	1.3
177	−11.7	−4.3	6.7	−61.9	−11.6
178	−16.4	−12.4	1.1	−85.8	−19.4
179	−30.1	−21.6	4.3	−33.2	0.9
180	−30.8	−22.8	4.4	−34.8	1.0
181	−12.5	−6.6	4.8	−32.8	5.8
182	−13.0	−7.3	4.4	−33.5	5.6
183	−22.5	−15.7	1.6	−35.1	−1.2
184	−14.9	−9.4	3.7	−27.1	2.5
185	−23.9	−18.7	0.9	−45.7	−1.6
186	−19.3	−13.4	3.0	−35.2	2.0
187	−16.4	−8.3	5.5	−78.2	−15.4
188	−33.1	−26.4	5.6	−40.0	2.0
189	−14.8	−7.4	5.4	−35.5	5.6
190	−26.9	−20.5	1.7	−49.3	−1.5
191	−21.0	−14.7	4.3	−37.9	2.4
192	−16.5	−8.2	6.7	−80.9	−14.8
193	−33.8	−27.4	5.6	−41.5	1.9
194	−15.3	−7.7	5.7	−37.1	6.2
195	−29.0	−21.3	0.7	−52.5	−2.4

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Table 29 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
196	−22.9	−15.1	3.5	−40.8	2.0
197	−17.5	−10.2	5.3	−84.9	−15.8
198	−36.0	−32.3	1.2	−43.9	−1.7
199	−17.2	−13.6	2.7	−39.9	3.2
200	−28.2	−23.9	−1.5	−53.4	−4.1
201	−26.2	−21.7	0.7	−43.4	0.1
202	−14.8	−7.1	5.7	−68.8	−15.0
203	−35.2	−27.0	4.4	−39.6	0.3
204	−14.7	−7.2	5.4	−30.0	4.5
205	−26.7	−18.8	0.4	−44.5	−3.1
206	−20.5	−12.5	4.1	−34.0	2.1
207	−16.5	−8.5	5.2	−79.1	−14.9
208	−33.7	−29.6	0.1	−38.5	−2.8
209	−16.9	−11.3	1.2	−36.4	2.1
210	−27.3	−21.9	−2.8	−48.6	−5.1
211	−19.8	−16.1	−0.3	−34.3	−1.6
212	−14.5	−7.1	5.1	−68.1	−15.1
213	−33.0	−24.9	4.6	−37.0	0.8
214	−14.6	−5.9	4.7	−32.5	5.0
215	−26.2	−18.3	0.0	−43.6	−2.6
216	−21.6	−13.7	1.2	−35.4	0.3
217	−15.2	−6.9	6.1	−74.2	−14.7
218	−36.2	−28.2	3.8	−41.3	−0.4
219	−16.7	−8.5	3.2	−36.3	3.4
220	−27.4	−19.5	0.2	−45.0	−3.0
221	−25.2	−16.9	1.9	−38.6	0.7
222	−18.4	−11.9	3.6	−82.9	−17.8
223	−35.7	−28.0	4.1	−41.1	0.0
224	−17.2	−13.0	3.2	−38.0	3.5
225	−25.7	−18.3	0.6	−41.8	−2.9
226	−22.9	−15.4	3.3	−39.5	1.0
227	−14.9	−7.0	4.8	−73.1	−15.2
228	−27.9	−21.0	4.5	−30.9	1.6

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Table 29 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
229	−15.1	−7.8	3.9	−30.5	3.1
230	−22.2	−15.9	1.2	−33.2	−2.3
231	−18.6	−8.7	1.5	−29.1	0.7
232	−14.5	−6.9	5.4	−73.6	−14.8
233	−33.7	−26.0	4.1	−38.6	0.8
234	−15.5	−7.4	3.2	−35.2	3.6
235	−27.5	−21.1	0.0	−44.4	−2.8
236	−19.0	−11.9	1.1	−31.7	0.2
MAXD	−46.4	−33.0	8.3	−86.8	−23.7
MD	−21.8	−15.5	2.4	−40.3	−1.9
MAD	21.8	15.5	3.7	40.3	5.2

Table 30: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the M06 functional. All values are without a counter poise correction. MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
1	−35.6	−29.4	−3.2	−32.6	−4.8
2	−42.4	−34.7	−5.4	−38.1	−7.5
3	−36.9	−30.5	−3.3	−33.6	−5.0
4	−44.1	−36.4	−5.9	−39.7	−8.2
5	−40.0	−33.2	−4.0	−36.5	−6.0
6	−45.7	−37.9	−6.8	−41.4	−9.2
7	−39.7	−33.2	−3.9	−36.5	−5.9
8	−23.8	−21.3	−8.7	−90.8	−27.5
9	−25.3	−23.0	−9.5	−93.2	−29.1
10	−25.3	−18.7	−4.2	−84.2	−24.0
11	−25.0	−19.4	−4.1	−85.3	−24.3
12	−23.1	−20.8	−7.8	−90.3	−26.9
13	−23.6	−21.4	−7.6	−91.5	−27.4
14	−24.8	−18.2	−3.7	−83.7	−23.6
15	−25.9	−20.5	−4.5	−88.2	−25.3
16	−22.7	−20.6	−6.8	−91.6	−26.6

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Table 30 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
17	−23.7	−21.6	−7.4	−91.7	−27.4
18	−24.2	−17.7	−2.9	−83.2	−23.1
19	−25.8	−20.6	−4.5	−88.6	−25.4
20	−22.5	−20.5	−6.5	−91.8	−26.3
21	−13.9	−13.9	1.1	−17.4	0.2
22	−18.6	−16.5	−0.1	−18.7	−2.1
23	−16.2	−16.5	−0.2	−19.1	−1.9
24	−14.8	−14.8	0.9	−18.1	−0.7
25	−17.3	−17.1	−0.9	−20.9	−2.4
26	−13.7	−13.6	1.8	−16.9	0.3
27	−13.8	−14.2	1.3	−17.6	−0.1
28	−12.7	−13.0	1.9	−15.9	0.8
29	−15.9	−16.2	0.3	−18.7	−1.6
30	−16.1	−15.9	0.8	−19.1	−1.1
31	−18.9	−17.4	0.1	−19.3	−2.5
32	−18.3	−18.3	−1.0	−21.4	−2.8
33	−11.4	−12.1	3.2	−15.0	1.8
34	−12.2	−12.7	2.3	−15.6	1.1
35	−14.6	−15.0	1.9	−17.5	−0.1
36	−16.8	−16.9	0.7	−19.9	−1.4
37	−10.0	−10.8	4.7	−13.6	3.2
38	−22.3	−22.6	0.3	−43.9	−4.4
39	−24.8	−23.5	−1.0	−48.9	−6.7
40	−22.4	−22.7	0.8	−44.5	−4.3
41	−26.9	−25.6	−1.6	−51.8	−7.8
42	−22.1	−22.5	1.2	−44.5	−4.0
43	−26.0	−24.8	−0.5	−51.2	−6.9
44	−22.6	−23.0	1.0	−45.0	−4.1
45	−23.2	−24.1	−0.3	−36.8	−0.1
46	−19.9	−22.4	0.8	−30.0	−1.9
47	−17.7	−18.9	−0.6	−28.7	1.1
48	−30.0	−30.8	−4.1	−43.6	−4.2
49	−26.5	−26.8	−0.7	−35.0	−2.8

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Table 30 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
50	−21.0	−21.5	−1.7	−32.8	−0.7
51	−23.5	−24.2	−0.2	−35.9	0.4
52	−30.6	−30.9	−3.4	−44.0	−3.5
53	−27.5	−27.6	−0.1	−36.0	−2.4
54	−21.1	−21.2	−0.9	−32.5	0.0
55	−21.4	−21.8	1.3	−33.0	2.2
56	−27.7	−19.6	−1.7	−33.5	−1.8
57	−35.7	−26.2	−5.2	−41.2	−5.2
58	−28.7	−20.5	−2.2	−34.4	−2.3
59	−29.8	−23.0	−3.6	−37.8	−3.8
60	−28.6	−20.7	−2.1	−34.6	−2.2
61	−38.6	−28.7	−6.0	−43.8	−6.4
62	−27.7	−19.9	−1.4	−33.8	−1.3
63	−20.4	−19.7	1.4	−42.9	−2.8
64	−50.9	−41.0	−7.5	−42.4	−10.7
65	−48.4	−39.0	−8.2	−39.1	−11.6
66	−50.9	−41.6	−7.6	−42.6	−11.3
67	−46.4	−38.8	−7.0	−38.9	−10.6
68	−48.2	−39.2	−7.8	−39.2	−11.4
69	−51.4	−42.6	−8.2	−43.6	−11.9
70	−47.0	−39.3	−7.3	−39.4	−10.8
71	−47.8	−39.3	−7.8	−39.2	−11.4
72	−51.2	−42.5	−7.9	−43.3	−11.8
73	−46.6	−39.0	−6.8	−39.3	−10.3
74	−48.0	−39.6	−7.8	−39.5	−11.5
75	−27.4	−21.7	−5.2	−90.1	−26.2
76	−25.8	−21.3	−4.6	−87.8	−25.6
77	−26.0	−22.0	−5.9	−86.6	−26.4
78	−25.9	−20.6	−3.8	−88.1	−24.8
79	−25.9	−21.8	−4.7	−87.8	−26.0
80	−24.7	−20.8	−4.7	−85.0	−25.2
81	−25.8	−20.7	−3.8	−87.9	−24.9
82	−25.1	−21.1	−4.0	−87.0	−25.2

Continued on next page

Table 30 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
83	−24.6	−20.6	−4.1	−85.5	−24.8
84	−25.0	−20.0	−2.9	−87.0	−24.0
85	−23.8	−21.4	−3.6	−25.7	−6.8
86	−22.9	−20.3	−3.8	−24.1	−7.2
87	−16.1	−16.0	1.7	−17.9	−1.8
88	−22.6	−19.7	−3.3	−23.0	−6.8
89	−22.4	−20.4	−2.7	−24.3	−5.9
90	−23.4	−21.3	−4.6	−23.5	−7.9
91	−22.4	−20.3	−2.7	−24.3	−5.9
92	−23.2	−21.2	−4.5	−23.3	−7.8
93	−21.8	−19.3	−2.6	−22.9	−6.2
94	−21.9	−19.4	−2.8	−23.1	−6.3
95	−22.7	−22.2	−4.5	−24.3	−7.6
96	−22.4	−20.3	−3.6	−22.4	−6.9
97	−22.9	−22.3	−4.6	−24.5	−7.6
98	−13.5	−14.0	3.4	−15.6	−0.1
99	−20.4	−18.8	−2.7	−21.5	−5.8
100	−20.7	−18.4	−1.5	−22.0	−5.2
101	−15.4	−14.2	0.3	−16.6	−3.0
102	−22.3	−20.2	−3.3	−22.5	−6.7
103	−22.8	−22.0	−4.3	−24.0	−7.6
104	−22.4	−20.2	−3.3	−22.6	−6.7
105	−19.5	−16.6	−0.2	−19.9	−4.0
106	−20.7	−18.3	−1.5	−22.0	−5.2
107	−32.4	−30.1	−4.8	−53.4	−12.1
108	−30.1	−28.2	−5.0	−50.3	−11.9
109	−32.6	−30.1	−4.3	−53.9	−11.8
110	−30.1	−28.4	−4.4	−49.5	−11.3
111	−30.1	−28.3	−4.6	−50.9	−11.8
112	−32.8	−30.3	−4.3	−54.3	−12.0
113	−29.4	−27.6	−3.6	−48.7	−10.5
114	−29.6	−28.2	−3.9	−50.5	−11.4
115	−32.4	−30.1	−4.0	−53.9	−11.8

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Table 30 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
116	−29.3	−27.7	−3.5	−49.0	−10.5
117	−29.5	−28.1	−3.7	−50.4	−11.3
118	−24.4	−25.4	−2.4	−34.7	−5.2
119	−18.3	−19.2	−1.2	−29.0	−2.2
120	−25.9	−28.1	−4.3	−35.6	−7.2
121	−21.0	−20.9	−2.1	−32.1	−3.4
122	−22.7	−24.3	−1.2	−34.1	−4.3
123	−17.7	−18.7	−0.1	−28.0	−1.1
124	−24.6	−26.3	−2.4	−36.3	−5.0
125	−20.9	−21.8	−2.6	−30.7	−3.8
126	−19.7	−20.1	−1.3	−29.6	−2.6
127	−23.2	−24.3	−0.2	−34.4	−3.0
128	−38.8	−27.3	−6.5	−41.0	−7.9
129	−37.8	−26.1	−7.3	−38.7	−8.8
130	−36.8	−26.4	−5.3	−39.3	−6.9
131	−36.5	−27.0	−6.6	−38.6	−8.1
132	−37.1	−25.9	−6.7	−38.3	−8.1
133	−39.0	−28.5	−7.0	−41.6	−8.7
134	−35.8	−26.4	−6.2	−37.9	−7.7
135	−36.9	−26.3	−6.7	−38.6	−8.2
136	−38.9	−28.2	−6.5	−41.4	−8.0
137	−35.4	−26.0	−5.7	−37.7	−7.2
138	−36.8	−26.2	−6.6	−38.5	−8.1
139	−27.6	−25.6	−3.3	−46.7	−8.8
140	−27.5	−25.3	−2.3	−46.8	−8.0
141	−25.1	−23.5	−2.6	−42.9	−7.7
142	−39.6	−33.5	2.1	−41.1	−8.6
143	−38.4	−32.9	0.9	−38.1	−9.4
144	−37.8	−32.7	0.7	−38.1	−9.0
145	−38.8	−32.6	1.5	−39.7	−9.0
146	−37.8	−32.2	0.2	−37.1	−10.0
147	−38.5	−32.2	0.3	−37.7	−9.4
148	−14.1	−9.2	1.9	−64.8	−15.6

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Table 30 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
149	−29.3	−25.5	−12.6	−98.5	−30.9
150	−31.7	−27.1	5.5	−34.5	−2.4
151	−26.3	−29.6	0.6	−35.4	−3.9
152	−17.0	−13.7	−0.8	−32.0	−3.7
153	−12.4	−14.7	−1.1	−31.5	−1.8
154	−23.4	−17.9	1.3	−37.9	−4.4
155	−22.4	−20.5	−1.7	−35.6	−4.7
156	−19.9	−18.0	−1.6	−39.5	−5.7
157	−20.7	−19.9	−0.7	−35.8	−2.3
158	−14.4	−9.7	1.9	−65.1	−15.7
159	−14.4	−9.8	1.8	−65.3	−15.9
160	−31.6	−27.2	5.7	−34.6	−2.3
161	−23.9	−27.6	3.0	−31.3	−1.4
162	−14.3	−10.5	3.0	−26.7	−0.4
163	−14.4	−13.5	0.7	−33.1	−1.0
164	−21.9	−17.0	2.9	−33.8	−2.7
165	−16.8	−13.5	2.4	−28.5	−1.8
166	−25.6	−22.8	−1.6	−46.5	−6.1
167	−23.5	−21.4	−1.2	−38.2	−4.5
168	−14.5	−9.7	2.2	−65.3	−15.5
169	−14.5	−9.8	2.1	−65.8	−15.6
170	−31.7	−27.0	5.1	−33.8	−3.0
171	−33.8	−32.6	3.1	−40.3	−4.6
172	−15.3	−10.4	2.1	−31.5	−1.2
173	−21.0	−19.7	−2.6	−40.2	−4.7
174	−17.6	−14.4	2.1	−29.1	−2.4
175	−29.1	−25.5	−1.0	−49.3	−6.3
176	−25.8	−22.5	−0.7	−41.5	−4.7
177	−13.9	−9.1	2.7	−64.4	−15.0
178	−28.3	−25.2	−10.7	−99.1	−30.2
179	−31.4	−26.7	5.4	−33.5	−2.7
180	−32.7	−28.3	4.8	−35.7	−3.3
181	−18.5	−15.0	0.4	−37.0	−2.1

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Table 30 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
182	−19.1	−15.9	−0.2	−38.1	−2.4
183	−20.9	−16.0	3.8	−32.8	−1.7
184	−17.0	−13.8	2.6	−28.3	−1.9
185	−26.7	−23.1	0.1	−46.6	−5.5
186	−23.2	−19.8	1.0	−37.7	−3.8
187	−20.7	−17.1	−2.7	−83.4	−24.4
188	−38.2	−37.1	1.5	−44.9	−8.4
189	−22.0	−18.4	−1.3	−41.6	−6.4
190	−30.1	−27.2	−1.4	−51.4	−9.5
191	−25.5	−23.5	−0.3	−41.9	−7.5
192	−22.7	−19.1	−3.8	−87.7	−26.1
193	−39.6	−38.7	0.8	−46.5	−9.4
194	−23.5	−19.9	−2.1	−44.0	−7.1
195	−32.8	−28.5	−2.5	−54.8	−10.9
196	−28.2	−24.7	−1.3	−45.0	−8.6
197	−25.1	−21.0	−3.8	−91.4	−25.5
198	−41.1	−41.5	−1.9	−47.9	−10.5
199	−23.5	−22.6	−2.8	−43.8	−6.5
200	−32.9	−30.6	−4.7	−55.5	−12.0
201	−31.8	−30.0	−4.2	−47.2	−8.6
202	−18.9	−15.9	−3.2	−73.6	−24.2
203	−39.0	−36.3	1.6	−42.8	−9.0
204	−18.7	−15.4	0.7	−33.4	−5.1
205	−27.6	−23.2	−0.4	−44.5	−8.8
206	−23.4	−20.1	1.0	−36.3	−6.3
207	−26.3	−21.1	−5.7	−87.6	−26.4
208	−38.7	−38.0	−2.1	−42.7	−10.2
209	−24.9	−22.3	−5.6	−42.1	−8.8
210	−32.2	−29.1	−5.8	−51.0	−12.5
211	−23.1	−21.1	−1.6	−36.2	−6.7
212	−17.3	−14.3	−1.9	−71.7	−21.8
213	−35.2	−32.5	3.8	−39.3	−5.9
214	−21.1	−15.7	−0.4	−38.5	−5.2

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Table 30 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
215	−27.9	−22.3	−0.1	−45.2	−7.2
216	−23.8	−19.4	0.1	−37.2	−5.6
217	−19.3	−15.3	−1.9	−78.3	−22.7
218	−39.4	−36.7	2.1	−44.1	−8.2
219	−22.2	−17.2	−1.0	−40.6	−6.1
220	−28.8	−24.2	−1.2	−45.0	−8.7
221	−29.3	−24.7	−1.5	−42.1	−7.1
222	−26.4	−22.5	−5.7	−89.6	−26.9
223	−38.5	−36.2	2.7	−43.4	−7.5
224	−24.9	−23.9	−4.3	−43.0	−7.4
225	−25.1	−20.8	1.4	−40.9	−6.6
226	−26.2	−22.7	0.1	−41.6	−7.5
227	−18.0	−14.0	−1.8	−76.6	−21.0
228	−32.2	−29.0	3.3	−35.4	−4.4
229	−19.6	−15.7	−0.3	−34.7	−4.7
230	−21.7	−18.1	1.3	−32.8	−4.4
231	−20.4	−13.1	2.6	−30.8	−3.2
232	−18.3	−14.3	−1.5	−77.4	−20.8
233	−38.1	−35.0	1.8	−42.4	−6.8
234	−21.5	−16.3	−1.2	−39.8	−5.1
235	−31.2	−26.5	−2.4	−47.3	−9.0
236	−21.9	−17.5	−0.1	−33.3	−4.7
MAXD	−51.4	−42.6	−12.6	−99.1	−30.9
MD	−26.6	−23.2	−2.0	−44.2	−8.9
MAD	26.6	23.2	3.1	44.2	9.0

Table 31: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the M06-2X functional. All values are without a counter poise correction. MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
1	−42.9	−35.9	−14.2	−39.9	−12.1
2	−48.3	−39.8	−15.5	−44.3	−13.4

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Table 31 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
3	−43.3	−36.0	−13.3	−40.3	−11.4
4	−49.4	−40.9	−15.4	−45.5	−13.5
5	−46.5	−38.9	−14.5	−43.4	−12.5
6	−50.5	−41.8	−15.9	−46.7	−14.0
7	−46.5	−39.0	−14.4	−43.6	−12.4
8	−16.2	−12.2	−1.2	−79.3	−20.2
9	−17.1	−13.0	−0.9	−81.9	−20.3
10	−20.7	−12.2	0.4	−77.5	−18.4
11	−20.1	−12.7	0.6	−78.2	−18.6
12	−16.0	−12.1	−0.6	−79.6	−19.8
13	−15.5	−11.5	0.8	−80.7	−18.7
14	−20.4	−11.9	0.7	−77.3	−18.1
15	−21.0	−13.8	0.2	−81.6	−19.6
16	−16.0	−12.5	−0.1	−81.3	−20.0
17	−15.5	−11.6	1.1	−80.8	−18.6
18	−20.1	−11.7	1.1	−77.3	−17.9
19	−21.4	−14.3	−0.1	−82.6	−20.0
20	−16.0	−12.6	0.0	−81.7	−19.9
21	−18.1	−16.6	−3.5	−20.6	−3.4
22	−16.4	−11.1	1.9	−16.1	1.9
23	−18.7	−17.0	−2.8	−20.7	−3.1
24	−18.9	−16.8	−3.3	−21.1	−3.5
25	−19.1	−17.1	−3.0	−21.9	−3.4
26	−17.7	−15.6	−2.6	−20.0	−2.9
27	−17.6	−16.2	−2.7	−20.5	−3.0
28	−17.7	−16.4	−3.2	−20.0	−3.4
29	−18.6	−16.8	−2.5	−20.5	−3.0
30	−20.8	−18.6	−3.9	−22.7	−4.3
31	−19.3	−15.1	−0.3	−19.7	−1.1
32	−20.7	−18.6	−3.4	−23.3	−3.8
33	−17.6	−16.4	−3.3	−20.4	−3.5
34	−17.4	−16.2	−2.9	−19.8	−3.2
35	−17.4	−15.6	−1.1	−19.5	−1.6

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Table 31 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
36	−19.4	−17.3	−1.8	−22.0	−2.4
37	−16.7	−15.6	−2.3	−19.4	−2.6
38	−30.4	−30.2	−9.1	−52.2	−11.3
39	−32.3	−30.2	−9.8	−56.7	−11.9
40	−30.6	−30.0	−8.5	−53.1	−10.8
41	−33.9	−31.7	−9.9	−59.3	−12.2
42	−30.4	−29.9	−8.1	−53.3	−10.4
43	−33.8	−31.8	−9.6	−59.6	−11.9
44	−30.7	−30.1	−8.0	−53.6	−10.4
45	−30.8	−30.6	−7.2	−43.7	−4.8
46	−19.5	−19.2	3.7	−30.0	3.4
47	−22.4	−22.6	−4.7	−33.2	−2.5
48	−34.8	−34.2	−8.3	−48.0	−5.9
49	−26.7	−24.5	1.1	−36.0	1.4
50	−25.2	−24.3	−5.1	−37.2	−2.9
51	−30.5	−29.7	−6.0	−42.7	−3.5
52	−36.1	−35.1	−8.2	−49.1	−5.8
53	−27.6	−25.3	1.5	−37.3	2.0
54	−25.6	−24.3	−4.4	−37.5	−2.3
55	−29.2	−28.1	−5.2	−40.5	−2.6
56	−35.0	−26.6	−12.1	−40.2	−9.3
57	−41.4	−31.6	−14.5	−46.5	−11.5
58	−35.6	−27.2	−12.4	−40.9	−9.6
59	−35.9	−28.3	−11.9	−43.4	−9.4
60	−35.6	−27.3	−12.2	−41.0	−9.4
61	−43.3	−33.2	−14.7	−48.7	−11.6
62	−35.5	−27.1	−12.1	−41.0	−9.2
63	−30.0	−28.7	−8.8	−53.0	−9.7
64	−51.7	−39.4	−11.4	−44.2	−10.4
65	−48.2	−35.9	−10.5	−40.0	−9.5
66	−51.6	−39.7	−11.1	−44.6	−10.3
67	−45.9	−35.6	−9.3	−39.1	−8.8
68	−47.6	−35.5	−9.5	−39.7	−8.7

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Table 31 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
69	−52.1	−40.8	−11.7	−45.6	−11.1
70	−46.9	−36.4	−9.7	−40.2	−9.0
71	−47.2	−35.7	−9.5	−39.8	−8.8
72	−51.7	−40.3	−11.1	−45.2	−10.5
73	−46.3	−35.9	−9.3	−39.9	−8.6
74	−47.4	−35.8	−9.5	−40.0	−8.7
75	−22.0	−13.0	0.8	−83.5	−18.4
76	−21.3	−13.4	0.9	−82.8	−18.5
77	−20.8	−13.7	0.3	−80.4	−18.8
78	−21.1	−12.5	1.6	−82.5	−17.6
79	−21.3	−13.6	1.0	−82.8	−18.6
80	−19.8	−12.8	1.3	−79.1	−17.8
81	−21.2	−12.7	1.6	−82.5	−17.7
82	−20.6	−12.9	1.7	−82.1	−17.9
83	−19.7	−12.5	1.9	−79.8	−17.4
84	−20.4	−11.9	2.5	−81.7	−16.9
85	−20.8	−16.2	−0.2	−22.1	−1.9
86	−21.3	−17.1	−2.5	−21.7	−4.1
87	−18.9	−16.0	1.0	−20.3	−0.9
88	−21.1	−16.5	−2.1	−21.0	−3.9
89	−20.0	−15.7	0.3	−21.4	−1.5
90	−20.3	−16.2	−1.6	−20.1	−3.3
91	−20.0	−15.7	0.3	−21.4	−1.5
92	−20.1	−16.0	−1.4	−19.9	−3.1
93	−20.7	−16.7	−1.9	−21.3	−3.6
94	−20.7	−16.6	−1.8	−21.2	−3.5
95	−18.1	−14.9	0.8	−19.5	−0.9
96	−19.3	−15.1	−0.5	−19.1	−2.3
97	−18.4	−15.2	0.7	−19.8	−1.1
98	−17.2	−15.0	1.7	−18.7	−0.6
99	−17.9	−14.4	−0.1	−18.7	−1.7
100	−19.6	−15.7	−0.7	−20.4	−2.5
101	−15.6	−12.9	0.0	−16.5	−1.9

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Table 31 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
102	−19.2	−15.0	−0.2	−19.2	−2.0
103	−18.5	−15.2	0.6	−19.6	−1.2
104	−19.1	−14.9	−0.1	−19.2	−2.0
105	−18.8	−14.4	0.1	−19.2	−2.0
106	−19.7	−15.7	−0.6	−20.4	−2.5
107	−32.6	−28.1	−6.3	−54.2	−9.5
108	−27.4	−22.4	−3.1	−48.1	−5.9
109	−33.3	−28.8	−6.5	−55.4	−9.9
110	−30.0	−26.7	−5.8	−49.9	−9.2
111	−27.9	−23.2	−3.3	−49.5	−6.4
112	−33.6	−29.1	−6.6	−56.1	−10.2
113	−29.6	−26.1	−5.3	−49.6	−8.7
114	−27.7	−23.2	−2.6	−49.5	−6.1
115	−33.1	−28.6	−6.1	−55.6	−9.7
116	−29.6	−26.2	−5.3	−49.9	−8.8
117	−27.4	−23.0	−2.3	−49.2	−5.8
118	−25.8	−24.5	−1.8	−36.3	−2.2
119	−20.1	−19.8	−2.5	−31.5	−1.9
120	−24.1	−23.2	−0.1	−34.0	−0.7
121	−22.7	−21.5	−3.6	−34.1	−3.0
122	−25.1	−24.6	−2.1	−37.1	−2.5
123	−20.0	−19.6	−1.5	−31.4	−0.9
124	−24.4	−24.2	−0.7	−36.9	−1.5
125	−21.4	−21.0	−2.5	−31.6	−2.2
126	−21.4	−20.6	−2.6	−32.1	−2.1
127	−25.9	−24.9	−1.3	−37.9	−1.6
128	−40.0	−26.8	−10.2	−42.8	−8.5
129	−38.1	−24.5	−9.6	−40.1	−8.0
130	−37.5	−25.3	−8.2	−40.8	−6.8
131	−36.3	−24.8	−8.4	−39.1	−7.2
132	−37.2	−24.0	−8.8	−39.6	−7.1
133	−40.0	−27.6	−10.2	−43.6	−8.7
134	−35.8	−24.2	−7.9	−38.5	−6.7

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Table 31 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
135	−36.9	−24.1	−8.8	−39.6	−7.2
136	−39.3	−26.8	−9.5	−42.8	−8.0
137	−35.4	−24.0	−7.7	−38.4	−6.5
138	−36.9	−24.1	−8.6	−39.6	−7.0
139	−28.7	−24.7	−5.0	−48.5	−7.1
140	−29.1	−25.1	−4.6	−49.6	−7.0
141	−26.1	−23.1	−4.5	−44.8	−6.8
142	−43.9	−33.7	−1.8	−44.4	−7.4
143	−42.5	−33.2	−2.9	−41.2	−8.6
144	−41.8	−33.8	−3.9	−41.4	−9.3
145	−41.8	−30.9	−0.7	−41.2	−5.6
146	−40.5	−30.5	−1.7	−38.3	−6.9
147	−41.2	−31.4	−2.7	−39.4	−7.6
148	−14.2	−7.2	2.7	−62.5	−14.2
149	−20.4	−15.6	−4.5	−84.5	−23.5
150	−34.5	−27.3	0.5	−37.4	−2.8
151	−30.0	−31.7	−5.8	−38.9	−6.8
152	−15.1	−10.2	−0.1	−30.0	−0.1
153	−12.8	−14.1	−1.9	−30.5	−1.7
154	−25.4	−18.5	−2.6	−40.1	−5.3
155	−23.4	−20.7	−4.7	−36.4	−4.8
156	−23.8	−21.5	−7.9	−43.4	−9.3
157	−24.4	−23.5	−5.9	−40.2	−5.5
158	−14.5	−7.5	2.9	−62.8	−14.1
159	−14.5	−7.5	2.9	−62.8	−14.2
160	−34.4	−27.3	0.9	−37.4	−2.6
161	−30.6	−32.4	−6.0	−37.3	−7.3
162	−16.4	−10.5	1.0	−28.5	0.5
163	−19.9	−17.9	−5.9	−39.0	−4.8
164	−26.1	−19.5	−2.0	−37.9	−4.7
165	−18.7	−13.5	−0.2	−30.4	−1.0
166	−29.1	−25.8	−7.3	−50.0	−9.3
167	−24.2	−20.8	−3.0	−38.7	−3.2

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Table 31 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
168	−14.7	−7.5	3.1	−63.1	−14.0
169	−14.6	−7.5	3.2	−63.4	−14.0
170	−34.8	−27.2	0.0	−37.0	−3.4
171	−34.4	−30.5	0.3	−41.0	−3.2
172	−16.0	−8.9	0.1	−32.0	0.4
173	−21.2	−18.5	−3.8	−40.4	−3.6
174	−19.5	−14.2	−0.3	−30.9	−1.1
175	−30.5	−26.1	−4.3	−51.5	−7.2
176	−27.3	−22.8	−3.9	−43.6	−4.5
177	−14.2	−7.0	3.6	−62.2	−13.4
178	−18.6	−14.5	−1.4	−85.3	−21.1
179	−34.7	−27.1	0.2	−36.8	−3.2
180	−35.4	−28.2	0.2	−38.5	−3.4
181	−18.8	−13.2	−0.8	−37.5	−0.1
182	−19.5	−14.2	−1.4	−38.6	−0.6
183	−25.5	−19.0	−1.4	−37.3	−4.0
184	−19.1	−13.8	0.1	−30.4	−0.8
185	−28.3	−23.5	−3.3	−48.9	−6.1
186	−24.4	−19.0	−1.6	−39.1	−2.6
187	−20.6	−12.4	1.0	−79.8	−19.0
188	−41.1	−35.1	−1.4	−46.8	−5.5
189	−23.0	−15.9	−1.8	−42.0	−2.1
190	−33.5	−27.4	−4.6	−54.4	−8.3
191	−28.2	−22.2	−2.2	−43.7	−4.2
192	−21.6	−13.0	1.3	−83.2	−19.2
193	−41.5	−35.8	−1.1	−47.9	−5.3
194	−23.8	−16.5	−1.8	−43.7	−1.8
195	−35.7	−28.2	−5.6	−57.6	−9.1
196	−30.1	−22.8	−3.1	−46.4	−4.7
197	−22.9	−15.5	−0.6	−88.3	−20.9
198	−44.6	−42.0	−6.7	−51.7	−10.5
199	−26.1	−23.2	−5.8	−47.2	−5.7
200	−36.4	−32.6	−9.5	−60.1	−12.8

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Table 31 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
201	−34.7	−31.3	−7.9	−50.5	−8.4
202	−19.2	−11.3	1.0	−70.2	−18.6
203	−41.9	−34.6	−1.5	−45.1	−6.1
204	−21.2	−13.9	−0.2	−35.2	−1.5
205	−31.7	−24.2	−4.3	−48.2	−8.2
206	−25.8	−18.3	−0.7	−38.1	−2.8
207	−21.7	−13.8	−0.6	−82.1	−20.0
208	−41.4	−38.5	−7.0	−45.3	−10.7
209	−24.3	−19.6	−5.9	−42.3	−5.7
210	−33.2	−28.6	−8.6	−52.9	−11.6
211	−27.2	−24.1	−7.2	−40.4	−8.7
212	−18.0	−10.7	0.9	−68.8	−18.0
213	−38.7	−31.5	−0.3	−41.9	−4.5
214	−21.4	−12.8	−1.1	−37.9	−1.3
215	−29.9	−21.9	−3.1	−46.3	−6.2
216	−26.8	−19.3	−3.3	−39.5	−4.1
217	−19.2	−11.0	1.4	−75.3	−18.2
218	−42.5	−35.4	−1.6	−46.6	−6.2
219	−25.0	−16.9	−3.9	−43.0	−4.1
220	−32.6	−24.9	−4.6	−48.9	−7.9
221	−31.1	−23.3	−3.5	−43.4	−4.5
222	−24.5	−18.0	−3.2	−87.0	−23.8
223	−41.7	−34.8	−1.0	−46.2	−5.5
224	−25.4	−22.0	−4.7	−44.6	−4.8
225	−30.1	−22.5	−3.1	−45.1	−6.9
226	−29.5	−22.4	−2.6	−44.6	−5.0
227	−18.3	−10.8	0.3	−73.8	−18.3
228	−32.5	−26.3	0.6	−35.0	−2.7
229	−20.7	−14.0	−1.3	−35.0	−2.3
230	−25.1	−19.4	−1.9	−35.5	−5.4
231	−22.4	−12.8	−1.4	−31.9	−2.3
232	−18.1	−10.8	0.9	−74.5	−17.9
233	−40.3	−33.8	−2.0	−44.2	−5.6

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Table 31 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
234	−23.5	−15.8	−3.9	−41.5	−3.8
235	−32.2	−25.9	−4.4	−47.8	−7.6
236	−23.6	−17.0	−2.9	−34.9	−3.4
MAXD	−52.1	−42.0	−15.9	−88.3	−23.8
MD	−27.7	−22.1	−3.6	−45.0	−7.7
MAD	27.7	22.1	4.1	45.0	7.8

Table 32: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the M08-SO functional. All values are without a counter poise correction. MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
1	−42.5	−35.6	−10.2	−40.1	−9.6
2	−48.2	−40.1	−11.7	−45.0	−11.4
3	−43.0	−36.1	−9.6	−40.7	−9.2
4	−49.2	−41.0	−11.4	−46.1	−11.3
5	−46.2	−39.1	−10.6	−43.9	−10.3
6	−50.1	−42.0	−11.8	−47.1	−11.9
7	−46.4	−39.3	−10.6	−44.2	−10.4
8	−21.2	−16.6	−5.9	−91.4	−26.2
9	−23.1	−18.8	−6.9	−95.7	−27.7
10	−22.0	−13.3	0.7	−86.5	−20.6
11	−22.1	−14.9	−0.6	−87.6	−21.9
12	−21.3	−17.0	−5.7	−92.2	−26.2
13	−21.6	−17.7	−5.4	−94.6	−26.3
14	−21.6	−13.1	1.0	−86.5	−20.3
15	−23.7	−17.0	−1.8	−91.7	−23.9
16	−20.9	−17.4	−5.0	−93.7	−26.5
17	−21.7	−17.9	−5.3	−94.9	−26.4
18	−21.2	−12.7	1.6	−86.4	−20.0
19	−24.0	−17.6	−2.3	−92.8	−24.5
20	−21.0	−17.7	−5.1	−94.3	−26.6
21	−20.9	−20.4	−5.5	−24.6	−4.6

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Table 32 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
22	−21.2	−16.5	−0.7	−22.7	−0.3
23	−21.9	−21.5	−5.2	−25.3	−4.9
24	−22.0	−21.0	−5.5	−25.7	−5.0
25	−22.5	−21.8	−5.7	−26.8	−5.5
26	−20.7	−19.8	−4.9	−24.4	−4.5
27	−20.7	−20.4	−4.9	−24.8	−4.5
28	−20.0	−19.9	−4.9	−23.4	−4.3
29	−21.8	−21.5	−4.9	−25.3	−4.8
30	−23.7	−23.0	−6.1	−27.2	−5.9
31	−23.0	−20.2	−3.2	−25.0	−3.4
32	−23.8	−23.2	−5.9	−27.8	−5.7
33	−19.7	−20.0	−5.0	−23.7	−4.6
34	−19.6	−19.6	−4.5	−23.1	−4.1
35	−20.6	−20.3	−3.5	−24.2	−3.4
36	−22.5	−22.0	−4.3	−26.5	−4.3
37	−18.7	−19.1	−4.0	−22.6	−3.7
38	−32.9	−33.7	−9.9	−57.0	−12.1
39	−34.7	−34.4	−11.4	−62.1	−13.8
40	−33.2	−33.9	−9.4	−58.2	−11.8
41	−37.0	−36.7	−12.2	−65.4	−14.7
42	−33.0	−33.8	−9.1	−58.5	−11.6
43	−36.8	−36.7	−11.8	−65.7	−14.3
44	−33.3	−34.2	−9.1	−58.7	−11.7
45	−32.9	−33.2	−8.0	−47.6	−5.9
46	−19.5	−20.4	4.7	−33.3	4.1
47	−23.9	−24.1	−4.6	−36.0	−2.7
48	−36.8	−37.4	−9.5	−52.2	−7.7
49	−27.6	−27.0	1.0	−40.1	0.9
50	−27.2	−26.3	−5.4	−40.7	−3.4
51	−32.7	−32.4	−6.5	−46.4	−4.3
52	−38.7	−39.2	−10.1	−53.9	−8.2
53	−29.1	−28.5	1.0	−42.0	0.8
54	−27.9	−26.5	−4.7	−41.3	−2.7

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Table 32 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
55	−31.0	−30.3	−5.4	−43.7	−3.0
56	−34.6	−25.9	−8.6	−41.4	−6.5
57	−41.3	−31.7	−11.3	−48.2	−9.4
58	−35.3	−26.9	−9.0	−42.2	−7.0
59	−36.3	−28.4	−8.7	−45.5	−7.4
60	−35.2	−27.0	−8.8	−42.4	−6.9
61	−42.7	−32.8	−10.7	−50.0	−9.0
62	−35.1	−26.7	−8.6	−42.2	−6.6
63	−32.4	−32.7	−10.8	−57.9	−11.6
64	−53.6	−41.6	−9.3	−46.6	−9.4
65	−49.3	−37.5	−8.3	−41.6	−8.3
66	−53.0	−41.6	−8.6	−46.6	−9.1
67	−48.7	−38.5	−7.5	−42.6	−8.4
68	−48.9	−37.4	−7.4	−41.6	−7.6
69	−53.4	−42.6	−9.1	−47.6	−9.7
70	−49.4	−39.1	−7.7	−43.5	−8.6
71	−48.6	−37.6	−7.2	−41.9	−7.5
72	−52.7	−42.0	−8.4	−47.0	−9.1
73	−48.8	−38.6	−7.2	−43.2	−8.1
74	−48.8	−37.7	−7.1	−42.1	−7.5
75	−28.4	−20.4	−6.0	−97.6	−26.8
76	−27.4	−20.9	−5.5	−96.6	−26.8
77	−26.0	−20.1	−5.1	−93.0	−26.0
78	−27.5	−20.1	−5.1	−96.6	−26.1
79	−27.3	−21.1	−5.3	−96.6	−27.0
80	−24.9	−19.3	−4.2	−91.8	−25.1
81	−27.4	−20.2	−5.0	−96.5	−26.2
82	−26.5	−20.4	−4.6	−95.8	−26.2
83	−25.0	−19.1	−3.6	−92.8	−24.8
84	−26.5	−19.5	−4.1	−95.7	−25.4
85	−25.5	−22.1	−4.3	−28.8	−5.2
86	−25.3	−22.7	−6.4	−27.4	−7.1
87	−21.5	−20.7	−2.2	−24.7	−3.7

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Table 32 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
88	−25.2	−21.9	−5.8	−26.5	−6.7
89	−24.5	−21.6	−3.6	−28.0	−4.7
90	−25.2	−22.1	−5.3	−26.7	−6.4
91	−24.5	−21.6	−3.6	−28.0	−4.7
92	−25.0	−21.9	−5.1	−26.5	−6.3
93	−24.7	−22.3	−5.8	−27.0	−6.7
94	−24.7	−22.2	−5.7	−26.9	−6.6
95	−22.6	−20.8	−2.7	−25.9	−4.2
96	−24.1	−21.0	−4.2	−25.6	−5.4
97	−22.8	−21.0	−2.8	−26.1	−4.4
98	−19.5	−19.3	−1.0	−22.7	−3.0
99	−21.8	−19.8	−3.7	−24.4	−4.6
100	−23.6	−21.3	−4.4	−26.1	−5.5
101	−18.4	−17.4	−2.6	−20.8	−4.0
102	−24.0	−20.9	−3.8	−25.8	−5.1
103	−22.9	−21.1	−3.0	−25.9	−4.6
104	−23.9	−20.8	−3.8	−25.7	−5.0
105	−22.8	−19.8	−3.4	−24.6	−4.8
106	−23.5	−21.2	−4.3	−26.0	−5.5
107	−36.7	−33.8	−8.2	−62.2	−12.0
108	−31.9	−28.2	−5.0	−56.7	−8.5
109	−37.4	−34.8	−8.5	−63.5	−12.6
110	−34.0	−32.2	−7.5	−57.6	−11.9
111	−31.9	−28.9	−5.0	−57.7	−8.8
112	−37.5	−35.2	−8.5	−64.1	−12.8
113	−33.5	−31.7	−7.0	−57.4	−11.4
114	−31.5	−28.8	−4.1	−57.6	−8.4
115	−36.8	−34.6	−8.0	−63.5	−12.2
116	−33.4	−31.7	−6.9	−57.6	−11.3
117	−31.2	−28.6	−3.8	−57.4	−8.1
118	−27.0	−28.0	−3.5	−40.6	−4.2
119	−21.8	−22.2	−3.2	−35.3	−2.6
120	−25.5	−26.9	−1.9	−38.6	−2.9

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Table 32 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
121	−25.4	−24.9	−5.2	−38.8	−4.7
122	−26.1	−27.7	−3.4	−41.2	−4.3
123	−21.6	−21.9	−1.8	−35.1	−1.6
124	−25.9	−27.6	−2.0	−41.1	−3.3
125	−23.3	−23.8	−3.3	−35.5	−3.6
126	−23.7	−23.7	−3.8	−36.5	−3.7
127	−27.5	−28.5	−2.8	−42.5	−3.8
128	−41.8	−28.7	−8.9	−46.2	−7.5
129	−39.1	−25.7	−8.3	−42.6	−6.7
130	−39.7	−27.3	−6.7	−44.4	−5.8
131	−38.7	−27.1	−7.5	−42.9	−6.8
132	−38.1	−25.2	−7.2	−42.0	−5.8
133	−40.9	−28.7	−7.9	−46.1	−7.1
134	−38.1	−26.5	−6.9	−42.3	−6.3
135	−37.6	−25.1	−6.8	−42.0	−5.6
136	−40.3	−28.1	−7.4	−45.5	−6.5
137	−37.7	−26.3	−6.5	−42.2	−5.9
138	−37.4	−25.1	−6.6	−41.9	−5.4
139	−32.7	−30.1	−7.2	−56.0	−9.5
140	−32.8	−30.5	−6.7	−57.0	−9.5
141	−29.9	−28.2	−6.5	−52.1	−9.3
142	−40.7	−31.5	5.0	−44.0	−2.2
143	−38.3	−29.8	5.0	−39.6	−2.3
144	−38.4	−30.6	3.6	−39.9	−3.0
145	−38.6	−29.2	5.6	−41.3	−0.8
146	−36.2	−27.4	5.8	−37.2	−1.0
147	−37.9	−28.8	4.2	−38.5	−1.7
148	−11.6	−3.4	7.5	−65.9	−11.6
149	−23.5	−16.7	−5.3	−94.8	−26.3
150	−31.8	−24.9	7.4	−37.1	3.5
151	−31.6	−34.5	−4.8	−42.4	−5.2
152	−17.0	−12.9	0.0	−34.9	0.3
153	−15.2	−16.6	−2.0	−35.4	−1.7

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Table 32 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
154	−24.4	−17.3	2.3	−41.9	−1.5
155	−26.2	−24.1	−5.2	−41.6	−5.4
156	−26.4	−24.9	−9.0	−48.5	−10.6
157	−26.2	−26.0	−6.0	−44.1	−5.9
158	−12.0	−4.0	7.5	−66.4	−11.8
159	−12.0	−4.0	7.4	−66.4	−11.9
160	−31.7	−25.1	7.7	−37.3	3.6
161	−31.2	−34.9	−5.1	−39.8	−5.5
162	−14.7	−9.2	5.5	−29.7	4.7
163	−21.2	−20.8	−6.1	−42.7	−4.6
164	−23.5	−16.7	4.1	−37.9	0.4
165	−15.7	−11.1	5.3	−30.4	3.6
166	−32.6	−29.9	−8.3	−56.5	−10.8
167	−25.8	−22.4	−1.7	−43.2	−2.3
168	−12.2	−4.1	7.7	−66.7	−11.7
169	−12.2	−4.1	7.6	−67.1	−11.7
170	−31.3	−24.3	7.4	−35.9	3.4
171	−33.3	−30.4	5.4	−42.4	1.6
172	−15.1	−9.1	3.6	−34.9	4.0
173	−24.5	−22.7	−4.9	−46.7	−4.4
174	−16.2	−11.6	5.4	−30.8	3.6
175	−32.3	−28.7	−3.1	−56.5	−6.7
176	−28.6	−25.5	−3.1	−48.0	−4.3
177	−11.6	−3.6	8.2	−65.8	−11.1
178	−23.5	−18.7	−5.2	−97.6	−27.0
179	−31.1	−24.2	7.7	−35.8	3.6
180	−32.7	−26.1	6.9	−38.4	2.8
181	−19.1	−14.5	1.7	−41.5	2.6
182	−20.2	−15.9	0.5	−42.8	1.7
183	−22.9	−16.1	4.7	−37.3	1.1
184	−15.8	−11.1	5.8	−30.2	4.0
185	−29.1	−24.9	−0.6	−52.9	−4.4
186	−24.2	−19.9	1.2	−42.3	−0.7

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Table 32 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
187	−17.4	−9.6	4.9	−85.4	−17.6
188	−37.3	−33.5	5.4	−47.1	0.6
189	−20.4	−15.6	2.3	−43.9	1.7
190	−30.8	−26.3	0.8	−56.1	−4.3
191	−24.9	−21.0	2.9	−44.9	−0.3
192	−18.3	−10.4	5.1	−89.3	−18.1
193	−38.3	−34.9	5.3	−48.8	0.2
194	−21.1	−16.1	2.9	−45.7	2.3
195	−33.0	−27.5	−0.2	−59.4	−5.4
196	−26.9	−22.1	2.2	−48.0	−1.1
197	−28.5	−23.1	−7.2	−101.8	−29.4
198	−47.9	−48.2	−8.9	−57.7	−12.1
199	−28.4	−27.8	−7.2	−53.0	−6.4
200	−39.4	−38.6	−12.2	−66.9	−15.5
201	−37.3	−36.2	−9.7	−56.3	−10.2
202	−14.5	−6.7	6.9	−73.9	−15.4
203	−38.0	−32.5	5.6	−45.1	0.2
204	−17.6	−11.9	5.1	−35.7	3.4
205	−28.2	−21.7	1.8	−48.6	−3.5
206	−22.1	−16.4	5.1	−38.7	1.8
207	−26.8	−20.1	−6.0	−94.1	−27.0
208	−44.6	−44.0	−8.6	−50.6	−11.8
209	−27.2	−24.2	−7.1	−48.3	−6.2
210	−37.1	−34.2	−10.6	−60.1	−13.9
211	−27.9	−27.0	−7.8	−43.9	−9.4
212	−14.3	−6.5	6.4	−72.7	−15.1
213	−34.8	−29.4	6.8	−41.4	2.2
214	−20.6	−13.8	1.9	−41.3	1.7
215	−30.3	−23.4	−0.8	−50.9	−4.6
216	−24.2	−18.4	1.3	−40.9	−0.2
217	−16.4	−8.0	5.5	−80.8	−16.4
218	−38.9	−33.9	5.2	−46.6	0.1
219	−22.9	−17.0	−0.2	−45.0	−0.4

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Table 32 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
220	−29.9	−23.4	0.4	−49.5	−3.6
221	−29.8	−23.7	0.0	−45.9	−1.9
222	−29.9	−25.3	−9.7	−100.1	−31.9
223	−38.2	−33.7	5.5	−46.3	0.5
224	−27.6	−26.3	−5.7	−50.1	−5.3
225	−27.0	−20.6	2.3	−45.7	−2.6
226	−26.2	−21.1	2.3	−45.6	−1.0
227	−16.1	−7.7	4.4	−79.1	−16.2
228	−32.6	−27.7	4.0	−37.5	0.7
229	−18.4	−12.7	3.3	−35.9	2.4
230	−22.0	−16.2	4.0	−34.9	0.0
231	−21.1	−12.8	2.2	−34.1	0.6
232	−16.5	−8.6	4.0	−80.4	−16.8
233	−38.0	−32.7	4.0	−44.8	0.4
234	−21.5	−15.5	−0.1	−43.3	0.5
235	−33.0	−26.7	−1.9	−51.6	−5.2
236	−21.0	−15.3	2.0	−35.6	0.8
MAXD	−53.6	−48.2	−12.2	−101.8	−31.9
MD	−28.9	−24.3	−3.0	−49.6	−7.8
MAD	28.9	24.3	5.5	49.6	8.4

Table 33: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the M08-HX functional. All values are without a counter poise correction. MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
1	−44.0	−37.1	−12.6	−41.1	−10.3
2	−49.8	−41.8	−14.4	−46.1	−12.2
3	−44.6	−37.5	−12.1	−41.8	−9.9
4	−50.7	−42.5	−14.0	−47.1	−11.9
5	−47.9	−40.6	−13.2	−45.0	−11.1
6	−51.7	−43.5	−14.6	−48.2	−12.5
7	−48.1	−40.8	−13.3	−45.4	−11.0

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Table 33 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
8	−16.7	−13.0	−4.1	−79.6	−20.3
9	−18.4	−14.9	−5.0	−83.3	−21.4
10	−21.8	−14.0	−2.6	−79.8	−19.6
11	−21.5	−14.9	−3.0	−80.6	−20.3
12	−16.7	−13.1	−3.8	−80.2	−20.1
13	−16.9	−13.5	−3.4	−82.1	−19.9
14	−21.5	−13.7	−2.3	−79.6	−19.3
15	−22.9	−16.5	−4.0	−84.2	−21.8
16	−16.6	−13.5	−3.3	−81.7	−20.3
17	−17.0	−13.7	−3.3	−82.4	−19.9
18	−21.1	−13.3	−1.6	−79.5	−18.9
19	−23.2	−17.0	−4.4	−85.2	−22.3
20	−16.7	−13.7	−3.5	−82.3	−20.4
21	−20.9	−20.2	−4.7	−23.8	−4.0
22	−20.0	−16.1	−0.9	−21.2	−1.1
23	−21.7	−21.3	−4.4	−24.5	−4.0
24	−22.1	−21.1	−5.1	−25.0	−4.7
25	−22.1	−21.7	−5.1	−25.9	−4.8
26	−20.3	−19.4	−4.0	−23.4	−3.6
27	−20.2	−19.9	−3.9	−23.7	−3.5
28	−20.2	−19.8	−4.3	−22.8	−3.7
29	−21.6	−21.3	−4.2	−24.4	−3.9
30	−24.3	−23.4	−5.8	−26.8	−5.4
31	−22.5	−19.9	−2.9	−24.1	−3.7
32	−23.3	−22.8	−4.9	−26.8	−4.5
33	−20.1	−19.9	−4.4	−23.2	−3.8
34	−20.0	−19.5	−4.0	−22.6	−3.5
35	−20.4	−20.1	−2.8	−23.3	−2.5
36	−22.2	−21.7	−3.4	−25.5	−3.1
37	−19.3	−19.0	−3.5	−22.3	−2.9
38	−32.4	−32.8	−9.4	−56.3	−11.1
39	−34.9	−34.1	−11.1	−62.0	−12.8
40	−32.6	−32.8	−9.0	−57.3	−10.6

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Table 33 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
41	−37.0	−36.1	−11.8	−65.2	−13.5
42	−32.5	−32.7	−8.7	−57.6	−10.3
43	−37.0	−36.3	−11.6	−65.7	−13.2
44	−32.7	−33.0	−8.7	−57.8	−10.3
45	−35.7	−36.1	−10.1	−49.8	−6.3
46	−21.2	−22.3	3.1	−34.1	2.3
47	−22.9	−23.9	−4.9	−34.8	−1.5
48	−38.6	−39.4	−11.2	−53.4	−7.4
49	−29.2	−28.8	−0.7	−40.9	−0.5
50	−26.8	−26.5	−6.3	−39.9	−2.7
51	−35.5	−35.2	−8.9	−48.4	−4.8
52	−40.7	−41.3	−11.8	−55.2	−7.7
53	−30.9	−30.4	−0.9	−42.8	−0.5
54	−27.9	−27.0	−5.7	−40.8	−1.9
55	−34.5	−33.7	−8.4	−46.2	−3.9
56	−36.7	−28.3	−12.0	−43.4	−7.8
57	−43.2	−34.0	−14.9	−50.2	−10.6
58	−37.4	−29.0	−12.5	−44.1	−8.1
59	−38.2	−30.9	−12.5	−47.4	−8.7
60	−37.4	−29.1	−12.4	−44.3	−8.0
61	−44.6	−35.0	−14.3	−52.0	−9.9
62	−37.5	−29.1	−12.4	−44.4	−7.9
63	−32.5	−32.6	−10.4	−57.9	−10.6
64	−54.1	−42.6	−11.7	−47.5	−11.3
65	−49.7	−38.4	−10.5	−42.4	−10.0
66	−53.3	−42.3	−10.8	−47.2	−10.5
67	−48.4	−38.8	−9.7	−42.4	−9.8
68	−49.0	−37.8	−9.3	−42.0	−8.9
69	−53.6	−43.1	−11.1	−48.0	−10.9
70	−49.3	−39.5	−10.1	−43.4	−9.9
71	−48.6	−37.9	−9.1	−42.0	−8.8
72	−53.0	−42.5	−10.5	−47.5	−10.2
73	−48.7	−39.1	−9.7	−43.0	−9.5

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Table 33 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
74	−48.7	−38.0	−9.1	−42.2	−8.7
75	−25.9	−18.1	−6.5	−89.1	−23.5
76	−24.4	−17.7	−5.4	−87.6	−22.7
77	−23.9	−18.1	−6.0	−84.8	−23.0
78	−24.8	−17.3	−5.4	−87.8	−22.4
79	−24.3	−17.8	−5.1	−87.5	−22.7
80	−22.9	−17.2	−5.0	−83.5	−22.1
81	−24.8	−17.4	−5.2	−87.7	−22.5
82	−23.6	−17.1	−4.4	−86.7	−22.0
83	−22.8	−16.7	−4.3	−84.3	−21.5
84	−24.0	−16.7	−4.4	−86.9	−21.6
85	−23.5	−21.4	−3.0	−26.7	−4.9
86	−24.8	−23.2	−6.2	−26.6	−8.0
87	−21.9	−20.8	−1.8	−24.9	−4.2
88	−24.3	−21.9	−5.2	−25.5	−7.2
89	−22.4	−20.6	−2.2	−25.8	−4.2
90	−23.5	−21.8	−4.7	−24.7	−6.5
91	−22.4	−20.6	−2.2	−25.8	−4.2
92	−23.3	−21.6	−4.5	−24.6	−6.3
93	−24.1	−22.6	−5.4	−26.1	−7.3
94	−24.0	−22.6	−5.3	−26.0	−7.3
95	−20.2	−19.5	−1.3	−23.1	−3.2
96	−22.5	−20.8	−3.7	−23.7	−5.4
97	−20.4	−19.8	−1.4	−23.4	−3.4
98	−20.2	−19.5	−1.0	−22.9	−3.6
99	−20.5	−19.4	−2.7	−22.5	−4.5
100	−23.0	−21.6	−4.0	−25.1	−6.2
101	−17.7	−17.2	−1.8	−19.7	−4.0
102	−22.4	−20.6	−3.3	−23.8	−5.2
103	−20.8	−20.2	−1.9	−23.4	−3.8
104	−22.3	−20.5	−3.2	−23.8	−5.1
105	−21.9	−19.6	−2.7	−23.4	−5.0
106	−23.0	−21.6	−4.0	−25.1	−6.1

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Table 33 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
107	−35.5	−32.7	−8.4	−60.8	−11.9
108	−30.0	−26.6	−4.8	−54.4	−8.1
109	−36.2	−33.5	−8.6	−62.0	−12.1
110	−33.3	−31.5	−8.3	−56.4	−12.1
111	−30.1	−27.2	−4.9	−55.4	−8.2
112	−36.2	−33.6	−8.4	−62.5	−12.0
113	−32.9	−31.0	−7.9	−56.1	−11.6
114	−29.7	−26.9	−3.9	−55.2	−7.6
115	−35.4	−32.8	−7.7	−61.8	−11.3
116	−32.8	−31.0	−7.7	−56.3	−11.5
117	−29.3	−26.7	−3.6	−54.9	−7.2
118	−29.0	−29.8	−4.9	−41.8	−5.5
119	−21.5	−22.5	−4.0	−35.0	−2.9
120	−25.7	−27.1	−2.1	−37.9	−3.1
121	−25.9	−26.1	−7.0	−38.9	−5.8
122	−27.6	−28.9	−4.5	−42.1	−4.9
123	−20.5	−21.3	−1.8	−34.0	−0.7
124	−27.2	−28.8	−3.6	−41.7	−4.4
125	−22.9	−24.0	−4.4	−34.6	−3.6
126	−23.8	−24.3	−5.1	−36.4	−4.0
127	−29.7	−30.5	−4.8	−43.9	−5.0
128	−42.1	−29.8	−11.6	−47.2	−9.3
129	−40.0	−27.2	−11.0	−44.2	−8.8
130	−39.4	−27.9	−9.1	−44.9	−7.2
131	−38.6	−27.8	−10.1	−43.3	−8.4
132	−38.7	−26.3	−10.0	−43.4	−7.6
133	−41.1	−29.4	−10.7	−46.9	−8.4
134	−38.0	−27.3	−9.6	−42.7	−7.8
135	−38.0	−26.1	−9.7	−43.0	−7.3
136	−40.2	−28.6	−10.0	−46.0	−7.6
137	−37.6	−27.0	−9.3	−42.6	−7.5
138	−37.9	−26.0	−9.6	−43.0	−7.1
139	−31.5	−29.5	−7.3	−54.7	−9.6

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Table 33 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
140	−31.4	−29.3	−6.4	−55.4	−8.8
141	−29.2	−28.0	−7.3	−50.9	−9.8
142	−43.4	−34.3	1.1	−46.6	−6.8
143	−41.6	−33.0	0.9	−42.6	−7.1
144	−41.7	−34.2	−0.5	−43.2	−7.9
145	−41.9	−32.4	1.6	−44.4	−5.8
146	−40.0	−31.0	1.6	−40.5	−6.1
147	−41.7	−32.7	0.0	−42.2	−7.1
148	−12.9	−5.8	2.6	−61.9	−12.8
149	−18.8	−13.4	−4.0	−81.5	−20.4
150	−34.1	−27.5	2.6	−39.0	−2.1
151	−31.9	−34.3	−6.2	−42.2	−4.9
152	−16.8	−13.1	−0.9	−33.8	−0.7
153	−14.0	−15.6	−1.5	−32.8	0.0
154	−25.0	−18.8	−0.4	−42.5	−4.5
155	−25.8	−23.8	−5.6	−40.4	−5.7
156	−24.8	−23.4	−7.8	−46.9	−9.1
157	−26.3	−26.4	−6.8	−44.4	−5.8
158	−13.2	−6.2	2.7	−62.3	−12.8
159	−13.2	−6.3	2.6	−62.3	−12.9
160	−34.1	−27.6	2.9	−39.1	−1.8
161	−32.6	−35.4	−6.7	−40.7	−5.9
162	−16.8	−11.7	1.9	−30.9	0.7
163	−21.9	−20.9	−6.7	−42.8	−4.3
164	−26.1	−19.8	−0.1	−40.3	−4.1
165	−18.5	−14.2	1.1	−32.7	−1.0
166	−30.9	−28.4	−7.7	−54.7	−9.5
167	−25.7	−23.0	−3.0	−42.6	−3.4
168	−13.4	−6.3	2.8	−62.6	−12.7
169	−13.3	−6.4	2.8	−62.9	−12.8
170	−34.5	−27.5	1.8	−38.7	−2.8
171	−34.3	−31.5	1.9	−43.0	−1.9
172	−16.4	−10.6	0.8	−35.2	1.0

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Table 33 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
173	−23.2	−21.6	−4.6	−44.0	−3.3
174	−19.0	−14.4	1.4	−32.9	−1.0
175	−31.7	−28.6	−4.3	−55.8	−7.7
176	−29.0	−25.8	−4.9	−48.3	−5.6
177	−12.9	−5.9	3.2	−61.8	−12.2
178	−18.7	−14.6	−3.4	−84.4	−20.4
179	−34.4	−27.4	1.9	−38.6	−2.7
180	−35.1	−28.6	1.9	−40.2	−2.7
181	−20.0	−15.6	−0.9	−41.4	0.1
182	−20.9	−16.8	−1.8	−42.6	−0.4
183	−25.6	−19.4	0.3	−39.7	−3.6
184	−18.6	−14.0	1.8	−32.3	−0.7
185	−28.8	−25.3	−2.5	−52.5	−6.1
186	−25.2	−21.1	−1.6	−43.1	−3.4
187	−18.0	−10.8	0.9	−78.9	−17.3
188	−39.5	−35.3	1.2	−48.2	−3.7
189	−22.7	−17.8	−1.1	−45.1	−1.6
190	−32.1	−27.7	−2.1	−57.0	−7.0
191	−27.4	−23.3	−0.9	−46.9	−4.0
192	−18.9	−11.6	1.0	−82.2	−17.7
193	−40.1	−36.4	1.2	−49.6	−3.8
194	−23.3	−18.2	−0.7	−46.6	−0.8
195	−34.5	−28.9	−3.3	−60.5	−8.1
196	−29.4	−24.2	−1.8	−49.9	−4.7
197	−26.1	−20.1	−7.3	−93.0	−25.5
198	−47.8	−47.1	−9.6	−57.2	−12.5
199	−29.7	−28.7	−9.0	−53.4	−7.5
200	−39.3	−37.8	−12.2	−66.6	−15.2
201	−38.2	−37.2	−11.4	−56.9	−11.2
202	−15.4	−8.1	2.7	−67.7	−15.2
203	−40.3	−34.4	1.4	−46.7	−4.3
204	−19.8	−14.0	2.0	−36.8	0.2
205	−30.0	−23.6	−1.1	−50.0	−6.4

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Table 33 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
206	−24.6	−18.5	1.5	−40.6	−2.0
207	−25.2	−18.5	−7.3	−86.5	−24.4
208	−45.1	−43.6	−10.1	−50.7	−13.0
209	−27.8	−24.5	−8.8	−47.8	−7.3
210	−36.5	−33.3	−11.1	−59.3	−14.0
211	−30.0	−28.3	−9.8	−45.7	−11.3
212	−15.2	−8.2	1.9	−67.1	−15.2
213	−37.3	−31.7	2.2	−43.4	−3.0
214	−22.1	−15.4	−1.0	−41.5	−1.3
215	−30.2	−23.9	−2.5	−50.4	−6.5
216	−26.6	−20.9	−2.2	−42.5	−4.1
217	−17.2	−9.5	1.2	−74.5	−16.3
218	−41.6	−36.1	0.5	−48.7	−5.0
219	−25.7	−19.4	−3.9	−46.7	−4.0
220	−31.4	−24.9	−2.0	−50.4	−6.1
221	−31.7	−25.8	−3.4	−46.9	−5.1
222	−28.0	−22.6	−9.9	−91.9	−28.3
223	−40.7	−35.6	1.0	−48.1	−4.3
224	−28.4	−26.5	−7.0	−49.9	−5.9
225	−28.7	−22.5	−0.6	−46.7	−5.4
226	−28.9	−23.3	−1.1	−47.8	−4.5
227	−16.9	−9.6	−0.1	−73.8	−16.5
228	−32.7	−27.9	1.5	−37.4	−2.6
229	−20.6	−15.0	0.2	−37.6	−1.2
230	−24.0	−18.8	0.8	−36.9	−3.6
231	−22.5	−14.2	−0.5	−35.5	−2.6
232	−17.2	−10.0	−0.1	−75.0	−16.7
233	−40.3	−35.0	−0.5	−46.7	−4.5
234	−24.2	−17.7	−3.5	−45.2	−3.0
235	−33.2	−27.7	−3.6	−51.4	−7.3
236	−23.4	−17.9	−1.5	−37.5	−2.9
MAXD	−54.1	−47.1	−14.9	−93.0	−28.3
MD	−29.2	−24.8	−4.6	−48.3	−8.4

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Table 33 – continued from previous page

N	6–31G**	6–311G**	6–311++G(3df,2p)	def2-SVP	def2-TZVP
MAD	29.2	24.8	5.2	48.3	8.5

Table 34: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the MP2 method. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−26.1	19.1	−1.2	11.2	−26.1	19.6	−13.7	7.9	−11.3	8.7	−5.3	4.3
2	−30.1	20.1	−2.1	11.0	−29.8	20.1	−16.2	7.8	−13.1	8.4	−6.7	4.1
3	−27.1	18.0	−2.5	10.5	−27.7	18.3	−14.6	7.6	−12.6	7.9	−5.8	4.2
4	−31.4	20.6	−2.7	11.3	−31.0	20.8	−17.0	8.0	−13.7	8.8	−7.0	4.3
5	−30.0	18.8	−2.7	10.6	−29.9	19.2	−16.2	7.5	−13.1	8.0	−6.8	4.0
6	−32.2	20.6	−2.3	11.4	−31.7	20.8	−17.9	7.9	−13.7	8.9	−7.3	4.3
7	−30.3	18.7	−3.1	10.8	−30.7	19.1	−16.7	7.4	−13.6	8.1	−7.0	4.0
8	−64.6	11.4	−66.4	6.9	−52.4	21.2	2.8	15.1	−13.4	6.9	0.8	6.9
9	−68.0	13.3	−66.2	7.8	−53.9	21.9	2.2	15.1	−14.2	7.0	0.1	6.7
10	−67.9	−4.0	−66.2	2.6	−61.4	4.6	4.1	15.0	−17.9	−1.0	−0.6	6.4
11	−67.4	−1.1	−65.9	3.4	−60.0	7.1	4.7	15.1	−17.2	0.2	0.0	6.7
12	−66.0	10.8	−66.4	6.6	−53.0	20.7	1.8	14.6	−13.6	6.4	0.2	6.6
13	−67.3	14.5	−65.4	9.1	−53.0	23.2	2.9	16.2	−13.3	8.3	1.1	7.9
14	−68.3	−4.1	−66.3	2.5	−61.6	4.5	3.5	14.9	−17.8	−0.9	−0.8	6.4
15	−70.3	2.8	−66.7	4.4	−60.7	10.0	3.6	14.9	−17.9	1.3	−0.7	6.4
16	−68.1	13.4	−66.9	8.1	−54.0	22.8	1.9	15.7	−13.7	7.9	1.1	7.8
17	−68.0	14.3	−66.0	9.0	−53.8	23.1	2.2	15.9	−13.8	8.2	0.6	7.7
18	−69.0	−3.7	−66.3	3.1	−61.6	5.2	3.1	14.8	−17.6	−0.3	−1.0	6.4
19	−71.2	3.8	−67.7	4.3	−61.5	10.4	2.5	14.3	−18.8	1.1	−1.5	5.9
20	−68.8	13.3	−67.4	8.0	−54.5	22.8	1.5	15.5	−14.2	7.9	0.8	7.7

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Table 34 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
21	−16.9	18.7	−7.1	3.5	−17.0	14.8	−15.1	3.9	−13.0	1.1	−10.8	−2.5
22	−17.9	10.4	−3.7	4.0	−21.1	5.1	−9.9	6.3	−13.4	−1.7	−8.3	−0.6
23	−19.9	16.8	−8.9	2.6	−20.6	12.5	−17.6	3.5	−15.4	−0.5	−12.6	−3.3
24	−18.2	17.5	−7.6	3.2	−19.5	13.2	−15.4	4.1	−14.6	0.1	−11.3	−2.6
25	−20.1	17.1	−8.7	2.6	−20.7	13.0	−17.2	3.3	−15.2	−0.5	−12.3	−3.3
26	−17.9	16.4	−8.1	2.4	−18.5	12.4	−16.3	3.3	−14.3	−0.4	−11.8	−3.1
27	−17.8	17.7	−7.9	2.9	−18.0	13.7	−16.5	3.5	−13.7	0.4	−11.5	−2.8
28	−17.2	18.2	−7.9	3.0	−17.6	14.2	−16.6	3.3	−13.5	0.8	−11.3	−2.8
29	−20.5	16.7	−9.5	2.3	−21.3	12.3	−19.0	3.2	−16.0	−0.7	−13.2	−3.5
30	−20.4	18.3	−9.0	2.6	−20.8	14.0	−18.9	3.1	−15.4	−0.1	−13.2	−3.5
31	−21.4	12.5	−6.5	2.9	−23.4	7.4	−15.2	4.5	−15.4	−1.9	−11.5	−2.2
32	−21.6	18.2	−10.1	2.6	−22.6	14.1	−18.8	3.1	−16.6	−0.3	−13.5	−3.7
33	−18.9	17.0	−9.7	2.2	−18.7	13.5	−18.1	3.0	−14.8	0.1	−12.3	−3.2
34	−17.6	17.9	−8.2	3.0	−17.8	14.2	−17.0	3.2	−13.7	0.8	−11.4	−2.7
35	−20.3	17.5	−8.9	3.2	−21.0	13.2	−18.8	4.0	−15.5	0.2	−12.7	−2.7
36	−21.0	19.8	−8.3	4.1	−20.9	15.9	−18.7	4.2	−14.9	1.3	−12.9	−2.6
37	−18.1	17.9	−8.7	3.2	−17.7	14.5	−17.5	3.9	−13.8	1.1	−11.4	−2.2
38	−43.8	18.7	−8.9	9.0	−37.6	20.9	−16.9	8.9	−18.6	6.7	−7.3	3.2
39	−48.8	20.7	−10.4	9.2	−42.1	21.8	−19.3	8.4	−21.2	6.2	−9.1	2.7
40	−45.4	18.0	−9.6	9.3	−39.4	20.3	−18.2	8.9	−19.1	7.0	−7.6	3.4
41	−51.3	21.6	−11.0	9.7	−44.8	22.7	−20.8	8.8	−22.2	6.7	−9.7	3.0
42	−46.1	17.7	−9.5	9.4	−39.6	20.3	−18.7	9.0	−18.9	7.2	−7.8	3.6

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Table 34 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
43	−52.0	21.8	−11.0	9.9	−45.1	23.0	−21.9	8.8	−22.2	7.0	−10.2	3.0
44	−46.6	17.3	−9.7	8.8	−40.3	19.8	−19.4	8.7	−19.3	6.6	−8.2	3.4
45	−42.4	11.1	−12.2	4.5	−41.4	11.2	−37.7	2.3	−21.5	0.9	−20.4	−2.4
46	−36.8	−2.9	−6.5	3.4	−39.0	−4.3	−23.5	4.2	−17.7	−2.0	−13.8	0.2
47	−26.7	12.5	−3.4	9.3	−30.5	11.1	−23.6	7.4	−13.5	4.5	−12.1	2.7
48	−47.1	13.1	−13.3	5.4	−45.9	13.1	−43.2	2.7	−23.5	1.4	−23.0	−2.3
49	−42.7	0.9	−8.8	4.1	−46.0	−1.1	−30.1	3.8	−20.7	−1.7	−17.4	−0.4
50	−31.1	12.9	−3.4	9.7	−34.9	11.2	−25.9	7.6	−14.5	4.6	−13.6	2.7
51	−40.3	11.1	−10.8	5.5	−40.8	11.4	−36.7	3.5	−20.9	2.0	−19.3	−1.2
52	−49.0	13.9	−14.7	5.3	−47.8	13.7	−46.6	2.6	−25.0	1.4	−24.6	−2.5
53	−45.0	2.2	−9.6	3.9	−48.7	0.4	−33.2	3.7	−21.7	−1.6	−19.1	−0.6
54	−32.8	13.1	−4.3	9.7	−36.8	11.3	−28.1	7.3	−15.7	4.3	−14.8	2.5
55	−39.1	11.0	−11.4	4.8	−40.0	11.4	−38.0	2.6	−20.8	1.3	−20.3	−1.8
56	−27.3	17.9	−3.2	11.0	−25.0	19.8	−16.3	7.9	−12.6	8.2	−7.5	4.0
57	−32.6	19.3	−4.2	11.2	−30.2	20.8	−19.6	7.8	−14.8	8.0	−9.6	3.7
58	−28.1	17.0	−4.1	10.3	−26.7	18.8	−17.8	7.4	−13.6	7.5	−8.3	3.7
59	−31.6	18.7	−4.8	10.4	−30.0	20.4	−20.3	7.2	−14.9	7.5	−10.1	3.1
60	−28.5	16.6	−4.3	10.0	−27.1	18.4	−18.4	7.3	−13.8	7.4	−8.6	3.7
61	−35.0	20.7	−5.0	11.9	−32.6	22.6	−22.4	8.0	−16.1	8.9	−11.0	3.8
62	−28.8	16.4	−4.1	10.0	−26.8	18.4	−18.8	7.2	−13.6	7.4	−8.8	3.6
63	−47.1	24.9	−8.1	11.5	−37.4	26.7	−24.7	8.1	−18.4	8.9	−11.1	2.8
64	−34.1	10.7	−3.3	7.4	−36.5	8.6	−15.7	5.0	−16.6	3.4	−8.2	2.2

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Table 34 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
65	−30.9	8.3	−3.1	5.8	−34.6	5.8	−14.8	4.1	−16.0	1.4	−8.1	1.5
66	−35.2	10.8	−4.0	7.5	−37.8	8.9	−17.2	4.9	−17.1	3.6	−8.7	2.2
67	−32.3	10.6	−3.4	6.7	−35.5	8.5	−15.7	4.8	−16.2	2.8	−7.9	1.9
68	−31.5	8.8	−2.7	6.7	−34.1	6.6	−15.6	4.6	−15.8	2.4	−8.2	1.9
69	−36.7	10.3	−5.2	6.5	−39.5	8.2	−18.7	4.2	−18.2	2.6	−9.6	1.5
70	−33.3	10.3	−3.4	6.7	−36.7	8.0	−16.7	4.6	−16.7	2.6	−8.5	1.8
71	−32.7	8.2	−4.7	5.8	−36.0	5.9	−17.1	3.9	−17.5	1.4	−9.1	1.4
72	−36.6	10.6	−4.9	7.4	−38.9	9.0	−18.7	4.6	−17.9	3.4	−9.5	1.9
73	−33.6	10.0	−3.5	6.6	−36.8	7.9	−17.3	4.5	−16.6	2.6	−8.7	1.8
74	−33.0	8.2	−4.7	5.8	−36.3	5.8	−17.4	4.0	−17.5	1.5	−9.2	1.4
75	−74.5	−6.8	−68.9	−0.2	−63.6	3.2	0.5	11.1	−20.5	−3.3	−3.0	3.4
76	−75.7	−5.8	−70.2	−0.5	−64.1	4.1	−2.5	9.8	−20.9	−3.2	−4.4	2.6
77	−73.3	−4.9	−68.9	−0.4	−62.8	3.9	−2.0	9.6	−20.3	−3.5	−4.4	2.4
78	−74.8	−6.8	−68.5	−0.3	−63.0	3.3	−0.7	10.7	−19.7	−3.2	−3.5	3.2
79	−76.4	−5.5	−71.2	−0.4	−65.3	4.5	−3.4	9.4	−21.8	−3.0	−4.8	2.4
80	−72.3	−3.7	−69.6	0.9	−63.4	5.4	−1.8	10.2	−20.8	−2.1	−3.8	3.2
81	−75.4	−6.8	−70.0	−0.7	−64.2	3.3	−1.7	10.1	−20.9	−3.4	−4.0	2.9
82	−75.8	−4.8	−70.9	0.2	−64.8	5.1	−3.0	9.9	−21.3	−2.4	−4.2	3.0
83	−73.9	−4.6	−70.0	0.8	−64.0	5.0	−2.3	10.2	−21.0	−2.0	−4.0	3.2
84	−74.7	−6.1	−69.3	0.3	−63.5	4.0	−1.2	10.8	−20.1	−2.4	−3.4	3.6
85	−19.0	10.4	−3.1	3.6	−19.9	6.5	−10.1	4.7	−10.8	−0.5	−7.4	−0.6
86	−17.9	11.3	−4.8	3.1	−20.7	6.4	−12.3	4.3	−12.3	−1.0	−8.3	−1.3

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Table 34 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
87	−22.2	2.8	−5.4	2.2	−23.2	1.3	−13.1	3.0	−13.1	−2.1	−9.0	−1.1
88	−17.4	10.8	−5.2	3.3	−20.2	6.3	−11.9	4.6	−12.4	−0.9	−7.9	−0.9
89	−19.7	9.9	−5.5	2.8	−21.4	6.0	−11.7	4.0	−12.8	−1.1	−8.2	−1.0
90	−18.6	11.6	−5.5	2.6	−20.9	6.6	−13.6	3.7	−13.0	−1.6	−9.2	−1.6
91	−19.7	9.9	−5.8	2.8	−22.1	6.0	−11.6	4.1	−13.1	−1.0	−8.2	−1.0
92	−18.4	11.7	−5.1	2.9	−20.7	6.8	−13.4	3.9	−12.6	−1.4	−9.0	−1.5
93	−18.5	11.1	−5.6	2.9	−21.4	6.2	−13.5	4.0	−12.9	−1.1	−8.8	−1.4
94	−18.5	11.1	−5.2	3.0	−21.2	6.3	−13.5	4.0	−12.6	−1.0	−8.7	−1.4
95	−19.0	11.6	−4.8	3.4	−21.2	7.4	−13.1	4.2	−12.2	−0.5	−8.1	−0.7
96	−17.9	12.4	−5.1	3.7	−20.5	7.5	−13.2	4.5	−12.7	−0.7	−8.5	−0.8
97	−19.1	11.9	−4.1	3.8	−20.7	7.9	−13.0	4.4	−11.6	−0.1	−7.9	−0.5
98	−21.9	3.4	−5.0	1.8	−22.4	1.5	−13.6	2.9	−12.5	−2.0	−8.9	−0.8
99	−17.0	11.6	−4.1	3.7	−18.8	7.2	−13.0	4.4	−11.3	−0.3	−8.0	−0.6
100	−18.4	11.6	−4.2	3.8	−20.1	7.1	−13.5	4.6	−11.3	−0.2	−8.2	−0.7
101	−16.9	10.6	−5.4	2.7	−18.1	6.1	−15.3	3.5	−11.7	−0.9	−8.8	−1.1
102	−18.6	11.7	−5.2	3.2	−20.8	6.9	−13.7	4.2	−12.7	−1.0	−8.8	−1.0
103	−19.0	12.3	−5.2	3.4	−21.1	8.0	−13.6	4.0	−12.5	−0.3	−8.4	−0.7
104	−18.6	11.8	−5.4	3.3	−20.8	7.0	−13.7	4.2	−12.9	−0.9	−8.8	−1.0
105	−18.2	10.7	−5.8	3.4	−20.6	6.4	−14.5	4.5	−12.7	−0.6	−8.6	−0.6
106	−18.5	11.4	−3.7	3.6	−19.7	6.8	−13.8	4.4	−10.8	−0.5	−8.4	−0.8
107	−51.2	9.2	−10.0	6.2	−49.8	8.1	−17.4	7.1	−23.2	1.2	−8.4	2.3
108	−47.9	4.7	−7.3	4.9	−45.8	3.3	−15.6	7.2	−20.7	−0.9	−7.6	2.1

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Table 34 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
109	−53.4	9.3	−10.7	5.8	−51.0	8.1	−19.9	6.7	−23.7	1.1	−9.3	2.1
110	−48.9	9.8	−9.7	5.8	−47.2	8.6	−18.0	6.8	−22.6	0.9	−8.4	2.1
111	−49.9	5.7	−9.5	5.0	−48.0	4.4	−17.5	6.9	−22.3	−0.5	−8.3	2.1
112	−54.7	9.7	−11.3	5.9	−51.7	8.8	−21.3	6.4	−24.1	1.4	−9.8	2.0
113	−49.2	9.9	−9.7	6.1	−47.2	8.7	−18.8	6.8	−22.5	1.2	−8.7	2.2
114	−50.9	6.1	−9.4	5.4	−48.2	5.1	−18.7	6.9	−22.4	0.1	−8.7	2.1
115	−54.6	9.8	−9.9	6.4	−50.3	9.2	−21.5	6.5	−22.6	1.8	−9.8	2.2
116	−50.1	9.2	−10.6	5.3	−48.4	8.0	−19.9	6.2	−23.4	0.5	−9.3	1.8
117	−51.1	6.1	−9.5	5.5	−48.5	5.0	−19.1	6.8	−22.7	0.1	−8.9	2.1
118	−41.9	−1.5	−10.5	1.2	−43.9	−2.9	−31.0	0.5	−20.7	−3.6	−17.3	−2.1
119	−31.8	3.4	−4.2	5.0	−35.2	1.9	−24.7	3.1	−14.8	0.2	−13.1	0.4
120	−40.4	−2.7	−9.3	1.5	−42.8	−4.1	−29.5	1.1	−20.0	−3.8	−16.5	−1.8
121	−32.9	3.9	−4.7	4.7	−37.0	2.2	−24.6	3.1	−15.3	−0.2	−13.2	0.2
122	−42.4	0.0	−9.2	1.8	−42.8	−1.2	−33.8	0.5	−19.4	−2.5	−17.8	−1.8
123	−32.9	3.8	−5.7	4.8	−36.9	2.4	−26.8	3.3	−15.8	0.3	−14.4	0.3
124	−44.2	−0.9	−10.4	1.7	−46.2	−2.4	−32.6	0.7	−21.2	−3.3	−17.7	−2.0
125	−31.9	6.0	−5.6	5.2	−37.8	4.1	−27.0	3.2	−16.4	0.5	−14.1	0.2
126	−32.1	4.1	−5.6	4.7	−37.3	2.7	−25.0	3.1	−16.0	0.0	−13.6	0.2
127	−44.6	0.0	−10.7	1.8	−46.1	−1.1	−35.4	0.4	−21.1	−2.8	−19.1	−2.1
128	−34.3	8.2	−4.9	6.4	−35.5	7.7	−18.7	4.2	−17.3	2.1	−10.9	1.3
129	−32.1	6.4	−4.8	4.9	−34.4	5.8	−17.7	3.4	−16.8	0.5	−10.6	0.8
130	−34.3	8.5	−4.8	6.6	−35.7	8.3	−19.5	4.5	−16.9	2.5	−11.0	1.5

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Table 34 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
131	−32.7	8.4	−3.8	6.4	−33.9	7.9	−18.5	4.2	−15.9	2.1	−10.5	1.4
132	−32.4	6.8	−3.9	5.6	−33.1	6.5	−18.9	3.7	−16.1	1.2	−10.9	1.2
133	−36.1	8.4	−7.2	5.9	−38.1	8.1	−21.9	3.7	−19.3	1.7	−12.4	1.0
134	−33.0	8.2	−4.7	5.7	−35.1	7.4	−19.5	3.8	−16.6	1.6	−11.0	1.2
135	−33.3	6.7	−5.9	5.1	−34.8	6.2	−20.2	3.4	−17.7	0.9	−11.6	0.9
136	−35.9	8.7	−6.0	6.4	−36.8	8.7	−22.1	4.0	−18.1	2.4	−12.4	1.3
137	−33.3	8.0	−4.8	5.7	−35.3	7.3	−20.3	3.7	−16.7	1.5	−11.4	1.1
138	−33.4	6.9	−6.0	5.3	−35.0	6.6	−20.5	3.6	−17.7	1.3	−11.7	1.1
139	−46.9	11.0	−6.3	8.1	−42.2	10.7	−19.5	6.9	−18.6	3.1	−8.9	2.4
140	−50.2	11.6	−7.8	8.1	−43.9	11.7	−23.7	6.2	−19.7	3.3	−10.4	2.2
141	−45.7	11.3	−7.0	7.1	−40.9	10.7	−21.6	6.2	−18.9	2.2	−9.6	2.0
142	−46.1	−3.6	−11.8	0.5	−50.6	−5.5	−8.8	6.7	−27.1	−6.1	−6.9	1.5
143	−41.3	−2.3	−10.2	1.4	−45.2	−4.4	−6.1	7.7	−25.2	−5.5	−4.9	2.2
144	−39.1	−1.1	−8.2	2.8	−42.6	−3.4	−4.5	8.9	−23.6	−4.8	−3.4	3.3
145	−44.0	−4.1	−10.9	0.6	−49.2	−6.8	−9.7	5.8	−26.2	−6.3	−7.5	1.0
146	−39.6	−3.0	−8.4	1.4	−43.2	−5.9	−7.1	6.6	−23.2	−5.7	−5.6	1.6
147	−37.9	−1.3	−7.3	3.2	−42.1	−4.4	−5.1	8.2	−22.9	−4.7	−3.9	2.9
148	−59.7	−15.2	−69.2	−5.2	−62.3	−5.7	2.1	10.4	−20.4	−7.9	−3.7	2.5
149	−65.3	2.5	−65.6	5.8	−52.6	17.9	7.4	20.1	−12.2	6.1	3.1	9.3
150	−36.7	0.3	−7.2	2.8	−46.6	−4.7	−4.2	9.1	−24.2	−5.2	−3.4	3.9
151	−33.5	15.1	−9.3	6.7	−35.0	15.5	−11.0	7.4	−21.7	3.8	−5.7	2.6
152	−28.0	9.0	−1.0	7.5	−27.9	7.2	−5.6	9.5	−12.9	2.3	−3.1	4.9

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Table 34 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
153	−30.5	11.0	−5.6	6.0	−25.6	13.9	−11.6	6.2	−13.5	4.6	−6.8	1.7
154	−38.3	4.0	−7.0	3.9	−38.5	1.2	−9.7	8.6	−18.8	−1.8	−5.6	2.8
155	−31.4	10.8	−2.9	8.3	−32.6	9.2	−11.7	8.6	−13.9	3.2	−5.2	4.0
156	−36.2	15.0	−4.8	8.6	−29.2	15.9	−12.2	8.7	−13.4	5.7	−4.6	4.0
157	−33.4	9.1	−5.7	6.9	−31.8	9.7	−14.6	7.0	−14.9	3.2	−7.1	2.8
158	−60.2	−15.7	−69.0	−5.0	−62.7	−6.2	1.9	10.4	−20.2	−7.8	−3.6	2.7
159	−60.1	−15.5	−69.0	−5.0	−62.6	−6.0	2.0	10.4	−20.2	−7.8	−3.5	2.7
160	−37.3	−0.4	−7.0	2.9	−46.7	−5.2	−4.5	9.0	−24.0	−5.1	−3.4	4.0
161	−32.8	16.3	−9.8	6.6	−35.2	15.8	−12.5	6.5	−22.9	3.1	−6.8	1.9
162	−30.1	0.7	−5.1	2.5	−33.3	−1.8	−8.9	6.3	−16.8	−3.3	−7.0	1.4
163	−34.3	12.2	−6.5	6.7	−28.6	13.9	−13.4	6.7	−16.7	3.7	−7.1	2.3
164	−37.8	0.0	−9.7	0.7	−41.7	−3.3	−11.6	5.5	−20.8	−5.0	−8.5	0.0
165	−32.5	1.2	−7.8	1.0	−36.3	−2.6	−15.3	3.9	−19.4	−5.2	−10.0	−0.5
166	−44.7	12.9	−8.7	7.5	−39.2	14.3	−15.0	8.4	−18.9	4.0	−6.6	3.1
167	−37.1	6.4	−5.1	6.1	−38.0	5.4	−15.6	7.1	−16.6	1.1	−8.2	2.5
168	−60.7	−16.0	−69.1	−5.1	−63.0	−6.4	1.7	10.3	−20.3	−7.9	−3.7	2.6
169	−60.8	−15.5	−69.1	−4.9	−62.8	−5.8	1.8	10.3	−20.2	−7.5	−3.5	2.7
170	−39.1	−2.8	−10.4	−0.6	−48.7	−8.3	−7.9	5.7	−27.1	−8.5	−6.5	0.8
171	−41.7	5.8	−9.5	4.7	−49.0	2.9	−8.0	8.8	−26.8	−2.2	−5.3	3.2
172	−33.3	6.3	−4.5	4.9	−31.5	4.6	−10.0	7.8	−17.4	−0.8	−6.5	2.8
173	−36.6	15.3	−3.6	9.6	−34.8	15.1	−11.6	9.6	−16.1	6.3	−6.0	4.7
174	−33.2	0.1	−8.1	0.4	−37.6	−4.0	−15.8	3.5	−19.6	−5.7	−10.3	−0.8

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Table 34 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
175	−48.4	12.5	−8.9	7.4	−46.9	12.2	−14.9	9.0	−21.7	2.7	−7.5	3.0
176	−42.2	12.7	−8.3	7.1	−41.4	10.6	−18.8	6.5	−20.6	1.6	−9.4	1.5
177	−60.1	−15.8	−68.9	−4.8	−62.6	−6.2	2.0	10.6	−20.1	−7.5	−3.3	3.0
178	−69.0	11.5	−65.8	9.1	−54.7	22.4	5.2	18.8	−13.2	8.7	2.8	9.5
179	−39.0	−2.8	−10.4	−0.5	−48.7	−8.1	−7.9	5.8	−27.0	−8.3	−6.4	1.0
180	−38.8	−1.8	−8.5	1.7	−48.2	−6.5	−5.9	7.8	−25.4	−6.2	−4.6	2.9
181	−38.7	9.5	−6.1	6.0	−37.7	8.3	−13.5	7.6	−20.0	0.7	−8.8	2.3
182	−38.9	10.8	−6.3	6.5	−37.9	9.8	−13.9	7.7	−19.9	1.5	−8.8	2.4
183	−37.5	−0.2	−9.2	0.9	−41.1	−3.3	−11.7	5.6	−20.3	−4.7	−8.4	0.3
184	−32.8	0.3	−8.1	0.7	−37.2	−3.8	−15.6	3.7	−19.5	−5.5	−10.0	−0.5
185	−47.1	11.0	−8.7	6.9	−45.8	9.7	−15.4	9.0	−21.5	1.8	−7.6	3.1
186	−40.2	9.4	−7.5	6.0	−41.2	5.6	−18.0	6.5	−20.2	−0.5	−9.1	1.6
187	−78.3	−13.3	−75.2	−4.7	−70.9	−2.2	−2.3	9.6	−26.1	−7.4	−6.6	1.3
188	−50.3	−0.2	−12.4	2.2	−57.0	−2.9	−12.2	6.9	−31.6	−6.0	−7.9	1.6
189	−45.3	6.7	−9.3	3.3	−44.4	5.5	−17.5	6.1	−24.8	−3.0	−11.9	0.2
190	−55.8	5.8	−13.2	3.9	−54.7	4.2	−19.0	7.3	−27.0	−2.3	−10.6	0.9
191	−47.9	4.4	−11.4	3.3	−49.3	0.7	−21.8	4.9	−25.0	−3.9	−12.1	−0.2
192	−82.7	−10.0	−76.3	−3.5	−73.0	0.3	−3.5	9.7	−27.2	−6.4	−7.1	1.4
193	−52.2	−0.7	−14.5	1.1	−60.1	−3.5	−13.5	6.3	−34.0	−6.7	−9.2	0.8
194	−48.6	6.5	−10.5	3.0	−47.5	5.4	−19.8	5.7	−26.3	−3.0	−13.3	−0.3
195	−59.3	5.3	−13.7	2.9	−58.1	3.4	−20.9	6.6	−28.4	−3.4	−12.3	0.0
196	−51.2	4.8	−12.4	2.5	−52.5	0.4	−23.5	4.5	−27.0	−5.0	−13.7	−1.1

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Table 34 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
197	−79.3	0.2	−71.7	1.0	−65.5	8.0	−2.7	10.2	−22.2	−1.9	−4.5	2.6
198	−48.3	7.0	−12.0	4.5	−55.2	5.2	−13.8	5.6	−30.2	−1.6	−8.1	1.5
199	−45.0	11.9	−8.3	6.5	−43.9	11.4	−19.4	6.1	−22.8	1.8	−11.6	1.3
200	−54.0	15.3	−11.1	7.8	−50.8	14.4	−20.8	7.7	−24.2	3.1	−10.1	2.3
201	−47.9	9.9	−10.2	5.7	−49.7	8.1	−25.8	4.8	−23.3	0.2	−13.5	0.5
202	−69.2	−14.5	−73.4	−4.6	−66.9	−2.6	−1.1	10.4	−24.3	−7.3	−5.7	2.1
203	−47.3	−0.8	−11.7	1.4	−54.9	−3.9	−9.8	7.7	−31.0	−6.8	−6.8	2.0
204	−39.0	2.1	−10.0	2.0	−40.8	1.0	−14.6	5.9	−23.9	−4.1	−10.1	0.3
205	−48.2	3.0	−10.6	3.1	−46.7	1.5	−15.1	7.5	−24.0	−3.1	−9.0	1.3
206	−41.9	2.5	−8.3	3.2	−43.5	−1.6	−16.8	5.7	−22.3	−4.6	−9.9	0.4
207	−72.2	0.0	−68.3	1.9	−62.1	7.9	0.3	11.9	−20.8	−2.1	−3.4	3.4
208	−39.7	8.7	−8.3	5.7	−46.5	6.4	−9.1	7.0	−25.5	−0.5	−5.2	2.8
209	−38.7	11.7	−5.2	7.0	−38.5	10.0	−15.3	6.9	−19.6	1.5	−9.2	2.0
210	−47.8	12.3	−8.9	7.1	−46.6	10.4	−17.0	7.9	−21.9	1.8	−7.9	2.4
211	−35.7	12.9	−6.3	7.1	−35.2	9.9	−17.6	5.9	−17.5	1.8	−8.0	1.9
212	−66.3	−15.2	−70.8	−4.5	−64.6	−3.6	1.6	11.6	−22.7	−7.4	−3.8	3.1
213	−42.8	−0.2	−8.4	3.2	−50.9	−3.8	−5.4	9.6	−27.8	−5.6	−3.5	4.2
214	−38.5	7.7	−4.9	6.3	−37.7	6.3	−10.4	8.9	−19.9	−0.4	−7.1	3.0
215	−44.3	3.0	−6.9	5.2	−44.8	1.4	−10.3	9.3	−20.8	−1.6	−5.9	3.0
216	−39.7	2.0	−7.3	3.3	−42.2	−1.0	−15.7	6.2	−21.6	−4.4	−9.7	0.9
217	−72.6	−12.4	−71.8	−3.4	−66.4	−1.3	0.7	11.8	−23.6	−6.5	−4.5	3.0
218	−48.6	−0.7	−11.5	1.8	−55.9	−4.0	−8.9	8.0	−31.2	−6.6	−6.0	2.4

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Table 34 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
219	−42.8	7.9	−9.4	4.3	−42.6	6.5	−14.4	7.3	−24.5	−2.1	−10.0	1.2
220	−48.2	3.0	−10.4	3.7	−47.5	1.7	−15.3	7.6	−23.7	−2.9	−9.2	1.4
221	−43.2	3.5	−7.6	4.0	−45.7	0.6	−18.4	6.3	−21.8	−3.3	−11.1	0.9
222	−74.8	7.4	−69.5	3.2	−62.6	12.4	−1.0	10.7	−20.8	−0.1	−3.3	3.2
223	−49.1	−1.4	−11.7	1.8	−56.4	−4.5	−9.5	7.7	−31.4	−6.6	−6.3	2.3
224	−41.9	12.8	−7.3	7.2	−42.4	11.4	−15.5	7.1	−22.2	2.1	−10.0	1.9
225	−46.0	0.4	−10.6	2.7	−45.7	−0.8	−14.4	6.9	−23.3	−3.7	−8.6	1.3
226	−47.4	4.1	−9.5	3.8	−47.4	0.4	−20.1	5.7	−23.7	−3.7	−11.2	0.4
227	−69.3	−12.7	−69.1	−2.9	−64.1	−1.8	3.7	13.0	−21.9	−6.7	−2.8	3.8
228	−34.4	0.5	−3.7	4.9	−40.8	−2.7	−0.8	9.4	−21.0	−3.2	0.1	5.4
229	−37.1	2.8	−6.5	3.5	−38.1	1.5	−8.6	6.6	−20.6	−3.1	−6.5	1.5
230	−35.2	0.1	−6.6	3.2	−34.8	−0.8	−7.9	6.8	−17.8	−2.9	−5.1	1.9
231	−32.0	5.1	−3.8	5.3	−33.4	−0.3	−9.9	7.6	−17.9	−3.4	−5.4	2.2
232	−70.1	−11.8	−69.3	−2.4	−64.1	−0.9	3.0	12.6	−21.8	−6.0	−2.7	3.9
233	−43.6	1.9	−7.9	4.8	−51.7	−1.4	−5.5	10.0	−27.8	−4.2	−3.2	4.5
234	−40.3	9.4	−6.5	6.0	−39.4	7.9	−11.4	8.7	−22.2	−0.8	−7.7	2.6
235	−45.0	3.5	−5.9	6.5	−44.7	2.7	−9.5	9.6	−20.1	−0.4	−5.6	3.3
236	−35.5	1.5	−6.0	3.4	−37.2	−1.4	−14.4	6.3	−19.4	−4.1	−8.5	1.2
MAXD	−82.7	24.9	−76.3	11.9	−73.0	26.7	−46.6	20.1	−34.0	8.9	−24.6	9.5
MD	−41.6	6.9	−18.0	4.4	−41.0	7.0	−13.8	7.0	−18.9	0.0	−8.3	1.7
MAD	41.6	9.4	18.0	4.9	41.0	8.6	14.4	7.0	18.9	3.3	8.4	2.4

Table 35: Deviation of interaction energy ΔE in kJ/mol to the corresponding reference structure N of the IL–2013 set for the SCS-MP2 method. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
1	−21.5	22.3	4.9	17.0	−21.3	22.9	−7.7	14.3	−4.9	14.5	1.0	11.3
2	−25.0	23.7	4.6	17.4	−24.5	23.8	−9.6	14.8	−5.9	14.7	0.1	11.7
3	−22.5	21.2	3.6	16.3	−22.9	21.7	−8.6	14.0	−6.1	13.7	0.4	11.1
4	−26.1	24.3	4.2	17.8	−25.6	24.5	−10.3	15.2	−6.4	15.3	0.0	12.1
5	−24.9	22.4	4.0	17.0	−24.6	22.9	−9.7	14.4	−6.0	14.4	0.0	11.5
6	−26.8	24.3	4.6	18.1	−26.2	24.7	−11.0	15.2	−6.4	15.6	−0.3	12.2
7	−25.2	22.3	3.5	17.0	−25.4	22.9	−10.2	14.4	−6.6	14.5	−0.2	11.5
8	−59.8	15.4	−55.9	14.6	−45.4	25.7	10.4	23.2	−5.5	14.4	8.9	15.7
9	−62.9	17.6	−55.6	15.7	−46.7	26.7	10.1	23.5	−6.0	14.9	8.5	15.9
10	−62.4	1.0	−56.6	9.6	−53.8	10.0	10.9	22.4	−10.4	6.5	6.4	14.3
11	−62.0	3.8	−56.2	10.5	−52.5	12.4	11.6	22.5	−9.7	7.6	7.1	14.6
12	−61.0	15.0	−55.9	14.5	−45.9	25.4	9.6	22.9	−5.6	14.3	8.5	15.6
13	−62.2	18.9	−6.7	17.1	−45.8	28.0	10.8	24.7	−5.0	16.3	9.5	17.2
14	−62.8	1.0	−56.7	9.6	−54.0	10.0	10.4	22.3	−10.3	6.5	6.2	14.3
15	−64.5	8.0	−8.5	12.1	−52.8	15.6	11.1	22.9	−9.8	9.2	7.0	15.0
16	−63.1	17.6	−8.2	16.2	−46.8	27.6	9.8	24.1	−5.5	15.9	9.5	17.0
17	−62.7	18.8	−55.1	17.1	−46.4	28.0	10.2	24.5	−5.4	16.3	9.2	17.1
18	−63.4	1.4	−8.6	10.2	−53.9	10.7	10.1	22.3	−10.0	7.2	6.1	14.4
19	−65.3	9.1	−9.2	12.2	−53.5	16.2	10.3	22.7	−10.4	9.3	6.5	14.8

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Table 35 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
20	−63.7	17.4	−56.5	16.1	−47.3	27.5	9.5	24.0	−5.9	15.9	9.3	17.0
21	−6.6	27.6	5.5	15.8	−6.5	24.4	−2.9	16.6	−0.3	13.4	1.9	10.9
22	−9.4	18.0	5.9	13.5	−12.3	13.3	−0.6	16.1	−3.4	8.1	1.3	9.7
23	−9.2	26.1	3.9	15.1	−9.7	22.4	−5.2	16.3	−2.5	12.1	0.3	10.3
24	−8.0	26.3	4.6	15.1	−9.0	22.7	−3.6	16.4	−2.3	12.1	1.0	10.4
25	−9.2	26.6	4.3	15.3	−9.6	23.2	−4.6	16.4	−2.1	12.3	0.7	10.5
26	−7.5	25.4	4.2	14.5	−7.9	22.1	−4.3	15.8	−1.8	11.8	0.5	10.0
27	−7.4	26.6	4.7	15.2	−7.3	23.4	−4.3	16.1	−1.0	12.8	1.2	10.6
28	−7.2	26.9	4.5	15.2	−7.2	23.7	−4.5	15.8	−1.1	12.9	1.2	10.5
29	−9.6	26.1	3.5	15.0	−10.3	22.4	−6.4	16.3	−2.9	12.0	−0.3	10.3
30	−9.4	27.7	4.1	15.5	−9.6	24.1	−6.2	16.4	−2.3	12.7	0.0	10.4
31	−11.3	21.3	5.0	14.2	−13.2	16.8	−4.0	16.2	−3.6	9.7	−0.1	10.1
32	−10.1	28.2	3.6	16.0	−10.8	24.8	−5.5	16.9	−2.9	13.2	0.2	10.9
33	−8.6	26.0	3.0	14.6	−8.0	23.2	−5.9	15.7	−2.1	12.5	0.3	10.2
34	−7.6	26.6	4.2	15.0	−7.5	23.5	−5.1	15.6	−1.3	12.9	1.0	10.5
35	−9.2	27.0	4.2	16.0	−9.8	23.4	−6.1	17.2	−2.2	13.1	0.4	11.3
36	−9.2	30.0	5.7	17.8	−8.9	26.8	−5.0	18.3	−0.8	15.0	1.1	12.3
37	−7.7	26.9	4.0	15.6	−7.1	24.1	−5.3	16.6	−1.1	13.5	1.2	11.2
38	−35.7	24.5	1.0	18.1	−29.4	27.0	−7.4	18.7	−8.4	15.8	2.3	13.6
39	−39.7	27.3	0.6	19.4	−32.9	28.7	−8.7	19.4	−9.8	16.5	1.6	14.3
40	−37.3	23.9	0.4	18.5	−31.1	26.4	−8.7	18.7	−8.9	16.2	1.9	13.9
41	−41.5	28.7	0.7	20.6	−34.9	30.2	−9.6	20.5	−10.1	17.7	1.5	15.3

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Table 35 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
42	−37.9	23.6	0.5	18.6	−31.3	26.4	−9.2	18.9	−8.7	16.4	1.8	14.1
43	−42.1	29.1	0.9	21.0	−35.1	30.6	−10.5	20.7	−10.0	18.1	1.3	15.5
44	−38.4	23.2	0.3	18.0	−32.0	25.9	−9.8	18.6	−9.1	15.8	1.4	13.9
45	−30.9	20.6	1.7	18.0	−29.4	21.2	−23.9	16.5	−7.2	14.4	−6.7	12.5
46	−28.8	4.0	2.1	11.8	−30.4	3.2	−14.9	13.2	−8.5	6.7	−5.6	9.3
47	−18.8	18.9	6.1	18.4	−22.2	17.7	−14.1	17.2	−3.4	13.8	−2.9	13.0
48	−34.4	23.5	1.8	20.0	−32.8	23.9	−28.0	18.3	−7.9	16.2	−8.2	14.0
49	−33.0	9.0	1.7	14.2	−35.7	7.6	−19.5	14.7	−9.5	8.8	−7.5	10.8
50	−22.4	19.9	6.7	19.5	−25.9	18.5	−15.6	18.3	−3.7	14.6	−3.6	13.9
51	−29.2	20.3	2.6	18.5	−29.3	21.0	−23.2	17.4	−6.9	15.0	−6.2	13.3
52	−35.6	24.8	1.2	20.7	−34.0	25.1	−30.7	19.0	−8.5	16.9	−9.2	14.5
53	−34.5	10.9	1.8	15.0	−37.6	9.6	−21.8	15.5	−9.7	9.7	−8.4	11.4
54	−23.7	20.3	6.2	19.8	−27.4	18.9	−17.4	18.4	−4.4	14.8	−4.4	14.1
55	−28.0	20.1	2.1	17.9	−28.5	21.0	−24.5	16.5	−6.8	14.5	−7.1	12.7
56	−21.9	21.6	3.6	17.1	−19.7	23.3	−9.7	14.8	−5.4	14.3	−0.7	11.5
57	−26.4	23.5	3.4	18.0	−24.0	24.9	−12.2	15.6	−6.7	15.0	−2.1	12.1
58	−22.7	20.6	2.7	16.4	−21.3	22.3	−11.3	14.3	−6.3	13.7	−1.6	11.2
59	−25.6	22.8	2.7	17.2	−24.0	24.6	−12.9	14.9	−6.9	14.5	−2.7	11.5
60	−23.2	20.2	2.5	16.2	−21.7	21.9	−11.8	14.2	−6.6	13.5	−1.9	11.1
61	−28.3	25.1	3.1	19.3	−26.0	26.9	−14.3	16.4	−7.4	16.4	−3.0	12.9
62	−23.5	20.0	2.6	16.2	−21.5	21.9	−12.3	14.0	−6.4	13.5	−2.2	11.0
63	−37.4	31.9	3.4	22.4	−27.8	34.0	−13.3	19.8	−6.5	19.7	0.1	15.2

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Table 35 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
64	−28.4	15.0	3.3	13.7	−30.6	13.2	−9.3	11.8	−9.4	9.8	−1.7	9.4
65	−25.6	12.3	3.0	11.6	−29.0	10.0	−9.0	10.2	−9.4	7.5	−2.2	8.1
66	−29.4	15.2	2.5	13.8	−31.8	13.5	−10.7	11.8	−9.9	10.1	−2.2	9.5
67	−26.9	14.8	3.0	12.8	−29.7	12.9	−9.6	11.3	−9.3	9.0	−1.8	8.8
68	−26.2	12.9	3.4	12.4	−28.5	10.9	−9.7	10.9	−9.0	8.4	−2.2	8.7
69	−30.9	14.7	1.6	12.8	−33.3	12.8	−12.1	11.2	−10.7	9.2	−3.1	8.9
70	−27.8	14.5	2.9	12.6	−30.9	12.4	−10.6	11.1	−9.7	8.8	−2.4	8.7
71	−27.3	12.4	1.6	11.6	−30.2	10.3	−11.1	10.3	−10.5	7.6	−3.1	8.2
72	−30.7	15.0	1.8	13.6	−32.9	13.5	−12.1	11.5	−10.6	10.0	−2.9	9.3
73	−28.1	14.2	2.8	12.6	−31.0	12.3	−11.1	11.0	−9.7	8.8	−2.6	8.7
74	−27.5	12.4	1.5	11.7	−30.4	10.3	−11.4	10.4	−10.6	7.7	−3.2	8.2
75	−68.3	−1.2	−10.3	7.8	−55.4	9.1	8.2	19.3	−12.0	4.9	5.0	12.2
76	−69.3	0.0	−59.0	8.0	−55.7	10.2	5.6	18.4	−12.0	5.4	3.9	11.8
77	−67.0	0.9	−58.0	7.7	−54.5	10.0	5.9	18.1	−11.7	4.8	3.8	11.4
78	−68.6	−1.1	−57.8	7.8	−54.9	9.2	7.1	18.9	−11.2	5.0	4.5	12.1
79	−70.0	0.3	−12.1	8.1	−56.8	10.7	4.7	18.1	−12.9	5.7	3.6	11.7
80	−66.0	2.0	−10.8	9.1	−55.1	11.4	6.1	18.7	−12.2	6.3	4.4	12.2
81	−69.2	−1.2	−11.2	7.6	−56.0	9.2	6.2	18.5	−12.3	5.0	4.1	11.8
82	−69.4	1.0	−11.7	8.7	−56.4	11.2	5.1	18.7	−12.4	6.3	4.2	12.3
83	−67.4	1.3	−58.9	9.1	−55.6	11.2	5.7	18.8	−12.3	6.4	4.2	12.3
84	−68.6	−0.5	−10.6	8.4	−55.4	10.0	6.6	19.1	−11.6	5.9	4.7	12.5
85	−10.6	17.7	6.2	12.7	−11.4	14.3	−1.0	14.2	−1.1	8.9	1.9	9.4

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Table 35 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
86	−9.2	18.8	5.0	12.7	−11.7	14.5	−2.8	14.2	−2.2	8.7	1.4	9.1
87	−15.2	8.8	2.7	10.2	−16.0	7.9	−5.0	11.4	−4.7	6.2	−1.0	7.7
88	−9.0	18.1	4.3	12.5	−11.6	14.1	−2.7	14.2	−2.6	8.6	1.5	9.1
89	−11.4	17.1	4.1	12.0	−12.8	13.7	−2.5	13.6	−2.9	8.4	1.1	8.9
90	−9.7	19.2	4.5	12.4	−11.9	14.7	−4.0	13.8	−2.7	8.3	0.7	8.9
91	−11.3	17.2	3.8	12.0	−13.5	13.8	−2.5	13.6	−3.3	8.4	1.2	9.0
92	−9.6	19.4	4.8	12.6	−11.6	14.9	−3.8	13.9	−2.3	8.6	0.8	9.0
93	−9.8	18.6	4.3	12.5	−12.4	14.3	−4.0	14.0	−2.6	8.7	1.0	9.1
94	−9.8	18.6	4.6	12.6	−12.2	14.4	−3.9	14.0	−2.4	8.8	1.0	9.1
95	−10.4	19.0	4.9	12.8	−12.4	15.3	−3.7	14.0	−2.1	9.3	1.5	9.5
96	−9.0	20.0	4.8	13.3	−11.5	15.6	−3.6	14.5	−2.3	9.3	1.3	9.7
97	−10.6	19.3	5.6	13.2	−11.9	15.7	−3.6	14.1	−1.6	9.6	1.6	9.7
98	−15.1	9.2	2.9	9.6	−15.4	7.8	−5.8	11.0	−4.3	5.9	−1.2	7.6
99	−8.7	18.7	5.2	12.8	−10.3	14.9	−3.8	14.0	−1.6	9.1	1.4	9.4
100	−9.6	19.1	5.8	13.4	−11.2	15.2	−3.9	14.6	−1.1	9.6	1.6	9.8
101	−8.9	17.3	3.6	11.4	−10.0	13.3	−6.6	12.6	−2.4	8.1	0.0	8.5
102	−9.8	19.4	4.8	12.8	−11.8	15.0	−4.1	14.2	−2.3	8.9	0.9	9.5
103	−10.4	19.7	4.6	12.9	−12.3	15.8	−4.2	13.9	−2.4	9.5	1.2	9.6
104	−9.8	19.4	4.6	13.0	−11.8	15.1	−4.1	14.3	−2.5	9.1	1.0	9.5
105	−9.7	18.0	3.7	12.6	−12.0	14.3	−5.3	14.1	−2.8	9.0	0.8	9.4
106	−9.8	18.9	6.2	13.1	−10.7	14.8	−4.2	14.4	−0.6	9.4	1.4	9.7
107	−42.6	15.6	−0.6	14.9	−41.0	14.8	−8.5	16.4	−13.1	10.3	0.4	12.1

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Table 35 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
108	−40.1	10.8	1.1	12.8	−37.8	9.6	−7.6	15.5	−11.6	7.4	0.3	10.8
109	−44.6	15.9	−1.0	14.8	−42.0	15.0	−10.7	16.2	−13.3	10.3	−0.4	12.1
110	−40.9	15.7	−0.8	14.0	−38.9	14.8	−9.6	15.5	−13.1	9.4	−0.2	11.2
111	−41.9	11.8	−0.7	13.1	−39.8	10.7	−9.4	15.4	−12.9	7.9	−0.3	11.0
112	−45.8	16.2	−1.5	14.9	−42.8	15.6	−12.1	16.0	−13.8	10.6	−0.8	12.0
113	−41.1	15.9	−0.7	14.2	−38.9	14.9	−10.5	15.5	−13.0	9.7	−0.5	11.3
114	−42.7	12.2	−0.5	13.6	−39.8	11.6	−10.4	15.6	−12.9	8.7	−0.5	11.2
115	−45.7	16.3	−0.2	15.3	−41.4	15.9	−12.3	16.1	−12.4	11.1	−0.8	12.2
116	−41.9	15.2	−1.5	13.5	−40.0	14.2	−11.5	15.0	−13.8	9.1	−1.1	11.0
117	−42.9	12.3	−0.5	13.7	−40.1	11.5	−10.8	15.5	−13.1	8.7	−0.7	11.2
118	−33.0	5.7	−0.9	10.4	−34.6	4.6	−21.5	10.3	−10.6	5.8	−8.3	8.0
119	−24.5	9.1	3.5	12.5	−27.8	7.9	−16.8	11.4	−6.3	7.9	−5.6	8.9
120	−31.6	4.5	0.1	10.4	−33.5	3.6	−20.1	10.7	−10.1	5.5	−7.7	8.1
121	−25.3	9.9	3.4	12.6	−29.2	8.4	−16.4	11.6	−6.6	7.8	−5.4	9.0
122	−33.4	7.3	0.5	11.3	−33.5	6.5	−24.0	10.7	−9.2	7.1	−8.6	8.6
123	−25.1	10.0	2.7	12.9	−29.0	8.8	−18.4	12.0	−6.8	8.5	−6.4	9.3
124	−35.1	6.4	−0.7	10.9	−36.7	5.4	−22.9	10.7	−10.8	6.3	−8.6	8.3
125	−24.0	12.3	3.0	13.5	−29.6	10.7	−18.3	12.3	−7.1	8.9	−5.9	9.6
126	−24.5	10.1	2.6	12.6	−29.5	8.9	−16.8	11.7	−7.2	8.0	−5.7	9.1
127	−35.1	7.7	−0.4	11.7	−36.2	6.9	−25.1	11.0	−10.1	7.3	−9.5	8.8
128	−28.3	12.5	1.6	12.4	−29.4	12.2	−12.3	10.9	−10.1	8.4	−4.7	8.5
129	−26.5	10.5	1.2	10.5	−28.7	9.9	−11.9	9.6	−10.1	6.4	−4.9	7.4

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Table 35 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
130	−28.2	12.9	1.8	12.8	−29.5	12.7	−12.9	11.3	−9.5	8.9	−4.6	8.8
131	−26.9	12.6	2.4	12.2	−28.0	12.2	−12.3	10.6	−9.0	8.2	−4.5	8.2
132	−26.8	10.9	2.2	11.3	−27.4	10.6	−12.9	10.0	−9.3	7.2	−5.1	7.8
133	−29.9	12.8	−0.3	12.2	−31.7	12.7	−15.2	10.7	−11.6	8.4	−6.0	8.4
134	−27.3	12.3	1.5	11.6	−29.1	11.7	−13.4	10.3	−9.6	7.7	−5.1	8.0
135	−27.6	10.8	0.3	10.9	−29.0	10.5	−14.1	9.8	−10.7	6.9	−5.7	7.7
136	−29.7	13.1	0.8	12.7	−30.5	13.1	−15.4	11.0	−10.6	9.0	−5.9	8.7
137	−27.6	12.2	1.5	11.6	−29.3	11.7	−14.1	10.2	−9.7	7.7	−5.5	7.9
138	−27.7	11.0	0.3	11.1	−29.1	10.7	−14.4	9.9	−10.7	7.2	−5.8	7.8
139	−38.6	17.2	2.7	16.5	−33.9	17.2	−10.7	16.0	−9.0	11.8	−0.4	12.0
140	−41.6	17.8	1.6	16.8	−35.3	18.3	−14.6	15.7	−9.8	12.4	−1.6	12.0
141	−37.9	17.0	1.6	15.0	−32.9	16.7	−13.4	14.7	−9.8	10.4	−1.6	10.9
142	−38.3	2.7	−3.7	8.3	−42.6	1.1	−1.3	14.5	−18.4	2.0	0.6	9.7
143	−34.4	3.1	−3.1	8.1	−38.3	1.3	0.4	14.5	−17.5	1.7	1.7	9.4
144	−32.7	3.9	−1.5	9.1	−36.1	1.9	1.6	15.3	−16.3	2.0	2.8	10.1
145	−36.2	2.2	−2.9	8.3	−41.2	−0.2	−2.3	13.5	−17.6	1.8	−0.1	9.1
146	−32.8	2.4	−1.5	8.0	−36.3	−0.2	−0.7	13.3	−15.7	1.3	0.9	8.7
147	−31.3	3.9	−0.5	9.6	−35.3	1.1	1.1	14.7	−15.5	2.0	2.4	9.8
148	−53.3	−9.0	−11.0	2.7	−53.9	0.8	9.4	18.2	−12.4	0.2	3.9	10.9
149	−62.1	4.9	−56.5	12.2	−46.8	21.2	13.5	26.7	−5.7	12.4	9.8	16.7
150	−29.5	6.3	0.3	10.0	−39.0	1.7	2.7	16.2	−16.0	2.4	3.5	11.5
151	−26.2	20.9	−0.2	15.0	−27.5	21.4	−2.5	16.3	−12.3	12.2	3.1	12.0

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Table 35 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
152	−22.0	13.8	5.3	13.5	−21.8	12.1	0.5	15.8	−6.1	8.7	3.0	11.6
153	−24.0	15.9	2.1	13.4	−19.2	19.0	−3.9	14.1	−5.6	11.9	1.0	10.1
154	−31.1	9.8	0.6	11.2	−31.1	7.3	−2.6	16.0	−10.7	5.7	1.5	10.6
155	−25.3	15.4	3.9	14.7	−26.3	13.9	−5.0	15.5	−6.6	9.9	1.3	11.3
156	−30.2	19.3	2.4	15.2	−23.2	20.4	−5.4	15.9	−6.1	12.4	2.4	11.7
157	−26.9	14.1	1.9	13.9	−25.1	14.7	−7.2	14.7	−6.9	10.3	0.3	11.0
158	−54.0	−9.6	−58.8	2.7	−54.4	0.2	9.1	18.0	−12.3	0.2	3.9	10.9
159	−53.8	−9.4	−10.8	2.7	−54.3	0.4	9.3	18.1	−12.2	0.3	4.0	11.0
160	−30.1	5.6	0.5	10.0	−39.2	1.2	2.3	16.0	−15.9	2.4	3.5	11.5
161	−24.8	22.7	0.0	15.6	−27.1	22.3	−3.4	16.1	−12.8	12.2	2.6	12.1
162	−22.7	7.1	2.5	10.0	−25.7	4.8	−1.6	13.9	−8.7	4.6	0.2	9.3
163	−27.1	17.7	2.0	14.6	−21.4	19.4	−5.3	15.0	−7.8	11.7	1.1	11.2
164	−30.0	6.6	−1.4	8.6	−33.6	3.6	−3.8	13.5	−12.1	3.3	−0.7	8.5
165	−24.7	8.0	0.5	9.1	−28.3	4.4	−7.3	12.2	−10.6	3.3	−2.1	8.1
166	−37.0	18.5	0.4	15.8	−31.3	20.2	−6.5	17.2	−9.5	12.4	2.0	12.4
167	−29.7	12.3	3.2	14.0	−30.3	11.6	−7.6	15.4	−7.8	9.2	−0.2	11.3
168	−54.5	−10.0	−11.0	2.6	−54.8	−0.1	8.9	17.9	−12.4	0.1	3.8	10.9
169	−54.5	−9.4	−10.9	2.9	−54.5	0.5	9.1	18.0	−12.2	0.5	4.0	11.0
170	−31.4	3.6	−2.5	7.0	−40.8	−1.4	−0.7	13.2	−18.5	−0.4	0.9	8.8
171	−33.3	12.5	−0.3	13.3	−40.4	10.0	0.5	17.7	−17.0	6.8	3.5	12.5
172	−25.6	12.7	3.6	12.6	−23.8	11.0	−2.2	15.8	−8.7	7.3	1.3	11.2
173	−29.3	20.6	4.6	17.3	−27.5	20.5	−3.7	17.8	−7.4	14.1	2.0	13.4

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Table 35 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
174	−25.5	6.7	0.1	8.4	−29.6	3.0	−8.0	11.5	−11.0	2.6	−2.6	7.7
175	−39.5	19.3	1.1	16.7	−37.7	19.3	−5.4	18.9	−11.2	12.3	2.0	13.3
176	−33.4	19.5	1.6	16.2	−32.4	17.7	−9.4	16.2	−10.3	11.1	0.0	11.8
177	−53.9	−9.7	−10.8	3.0	−54.4	0.1	9.2	18.2	−12.2	0.4	4.1	11.2
178	−64.9	14.7	−56.1	16.1	−48.2	26.3	12.1	26.2	−5.9	15.6	10.2	17.6
179	−31.4	3.7	−2.4	7.2	−40.7	−1.3	−0.6	13.3	−18.5	−0.3	1.0	9.0
180	−31.6	4.2	−1.0	8.8	−40.7	−0.2	0.9	14.9	−17.3	1.3	2.3	10.4
181	−29.6	16.9	3.8	15.3	−28.5	15.8	−4.1	17.3	−9.6	10.4	0.6	12.5
182	−29.7	18.2	3.8	16.0	−28.6	17.3	−4.3	17.5	−9.3	11.3	0.8	12.9
183	−29.8	6.4	−0.9	8.9	−33.0	3.5	−3.9	13.7	−11.6	3.6	−0.6	8.8
184	−25.1	6.9	0.1	8.6	−29.3	3.1	−7.8	11.7	−10.9	2.8	−2.3	7.9
185	−38.3	17.8	1.1	16.0	−36.7	16.8	−6.1	18.7	−11.2	11.2	1.6	13.2
186	−31.7	16.2	1.9	14.6	−32.4	12.7	−9.1	15.7	−10.4	8.6	−0.4	11.2
187	−70.5	−6.0	−14.8	5.3	−61.0	5.6	6.9	19.4	−16.0	2.7	3.0	11.9
188	−41.4	7.1	−2.7	11.5	−47.9	4.6	−3.2	16.2	−21.2	3.7	1.2	11.5
189	−34.9	15.3	1.9	14.2	−33.8	14.3	−6.8	17.2	−12.9	8.3	−1.1	11.9
190	−45.6	13.9	−2.1	14.5	−44.2	12.6	−8.5	18.2	−15.3	8.6	−0.2	12.3
191	−38.2	12.4	−0.9	13.4	−39.2	9.1	−11.8	15.3	−13.9	6.6	−2.2	10.6
192	−74.6	−2.5	−63.4	6.9	−62.7	8.2	6.2	20.0	−16.6	4.1	2.9	12.5
193	−43.0	6.8	−4.5	10.7	−50.6	4.3	−4.3	15.9	−23.3	3.1	0.1	10.9
194	−37.7	15.5	1.1	14.3	−36.5	14.6	−8.6	17.2	−14.0	8.5	−2.1	11.8
195	−48.8	13.5	−2.4	13.7	−47.3	12.0	−10.2	17.7	−16.5	7.7	−1.7	11.7

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Table 35 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
196	−41.0	13.0	−1.5	12.8	−42.0	9.1	−13.2	15.1	−15.5	5.7	−3.6	10.1
197	−72.5	6.2	−11.9	10.0	−24.7	14.4	6.0	19.4	−12.7	7.2	4.5	12.5
198	−40.4	13.0	−2.8	13.0	−47.0	11.5	−5.3	14.5	−20.4	7.1	0.5	10.8
199	−35.5	19.3	2.4	16.5	−34.3	18.8	−9.3	16.6	−11.5	12.0	−1.4	12.4
200	−44.6	22.3	−0.3	17.7	−41.1	21.6	−10.5	18.3	−12.8	13.3	0.1	13.5
201	−38.6	17.0	0.2	15.4	−40.1	15.5	−15.7	15.2	−12.2	10.3	−3.6	11.4
202	−62.0	−7.7	−13.8	4.6	−57.6	4.6	7.5	19.5	−14.9	2.2	3.2	12.0
203	−38.7	6.2	−2.5	10.2	−46.1	3.5	−1.4	16.4	−21.1	2.4	1.7	11.3
204	−29.8	9.9	−0.2	11.5	−31.4	9.0	−5.3	15.5	−13.4	5.8	−0.8	10.4
205	−39.4	10.2	−1.0	12.3	−37.7	9.0	−6.1	16.9	−13.8	6.4	0.0	11.2
206	−33.3	9.6	0.8	11.9	−34.6	5.9	−8.2	14.7	−12.5	4.6	−1.3	9.8
207	−65.7	5.9	−57.1	10.4	−53.6	14.0	8.5	20.6	−11.8	6.7	5.1	12.8
208	−33.0	13.7	−0.7	12.8	−39.6	11.7	−2.0	14.5	−17.2	6.9	2.1	10.7
209	−30.3	18.3	3.9	15.6	−30.0	16.7	−6.5	16.0	−9.7	10.6	−0.3	11.7
210	−39.7	18.2	0.1	15.3	−38.2	16.6	−8.6	16.7	−12.4	10.3	0.4	11.7
211	−28.8	18.1	1.5	14.3	−28.1	15.3	−10.2	13.7	−9.4	9.2	−0.7	10.1
212	−59.8	−9.0	−60.1	3.8	−56.1	3.0	9.2	19.7	−14.3	1.1	4.1	12.0
213	−35.4	5.8	−0.6	10.7	−43.2	2.5	1.7	17.0	−19.2	2.3	3.8	12.1
214	−29.5	15.1	4.6	15.4	−28.6	13.9	−1.3	18.3	−9.6	9.2	2.2	13.0
215	−36.5	9.4	1.6	13.4	−36.6	8.1	−2.4	17.5	−11.6	7.0	2.1	11.8
216	−31.5	8.8	1.3	11.6	−33.9	6.1	−7.5	14.7	−12.3	4.4	−1.5	10.0
217	−65.8	−5.9	−12.5	5.5	−57.4	5.6	9.0	20.6	−14.4	2.6	4.1	12.5

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Table 35 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
218	−40.7	5.7	−3.0	9.8	−47.7	2.7	−1.2	15.9	−21.9	1.9	1.9	10.9
219	−33.1	15.8	1.1	14.3	−32.8	14.5	−4.5	17.5	−13.3	8.3	0.0	12.1
220	−39.3	10.2	−0.8	12.8	−38.4	9.2	−6.3	16.9	−13.5	6.7	−0.1	11.4
221	−34.2	10.8	2.0	13.4	−36.5	8.2	−9.1	15.8	−11.6	6.5	−1.9	11.0
222	−68.0	13.4	−9.8	12.2	−53.8	18.7	7.8	20.1	−11.2	9.0	5.9	13.3
223	−41.2	4.9	−3.3	9.7	−48.3	2.2	−1.9	15.7	−22.2	1.8	1.5	10.8
224	−32.5	20.2	3.0	17.0	−32.9	19.0	−5.5	17.5	−11.1	12.2	0.0	12.8
225	−38.2	6.6	−2.2	10.6	−37.8	5.6	−6.6	15.1	−14.3	4.6	−0.7	10.0
226	−38.3	11.4	0.2	13.1	−38.1	8.1	−10.9	15.3	−13.4	6.0	−2.1	10.5
227	−63.0	−6.7	−10.7	5.3	−55.9	4.5	11.2	21.0	−13.6	1.7	5.1	12.5
228	−29.1	4.7	1.9	10.1	−35.2	1.7	4.0	14.5	−14.7	2.4	5.2	11.0
229	−29.3	9.2	1.5	11.2	−30.2	8.0	−1.0	14.5	−11.9	5.1	1.2	9.8
230	−29.2	5.0	−0.3	9.2	−28.7	4.2	−2.1	13.0	−11.0	3.5	0.8	8.4
231	−25.4	10.5	3.0	11.7	−26.6	5.4	−3.6	14.2	−10.5	3.6	1.0	9.2
232	−64.0	−6.0	−11.0	5.6	−56.0	5.1	10.5	20.5	−13.6	2.2	5.0	12.5
233	−36.5	7.6	−0.3	12.0	−44.4	4.5	1.4	17.2	−19.5	3.4	3.9	12.2
234	−31.3	16.7	3.2	15.3	−30.2	15.3	−2.2	18.1	−11.7	8.9	1.6	12.6
235	−37.3	9.5	2.2	14.1	−36.9	8.8	−1.9	17.6	−11.4	7.7	2.1	11.8
236	−28.4	7.4	1.5	10.6	−29.9	4.7	−7.2	13.7	−11.2	3.6	−1.3	9.1
MAXD	−74.6	31.9	−63.4	22.4	−62.7	34.0	−30.7	26.7	−23.3	19.7	10.2	17.6
MD	−33.9	13.2	−3.9	12.9	−32.7	13.6	−5.2	15.9	−9.6	8.8	0.3	11.1

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Table 35 – continued from previous page

N	def2-SVP		def2-TZVP		cc-pVDZ		aug-cc-pVDZ		cc-pVTZ		aug-cc-pVTZ	
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}
MAD	33.9	14.1	7.5	12.9	32.7	13.6	8.4	15.9	9.6	8.8	2.8	11.1

Table 36: Deviation of interaction energy ΔE in kJ/mol to the reference values of the IL–2013 set of selected GGA and meta-GGA functionals in combination with the 6–31++G** basis set. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation;

	BLYP-D3		BP86-D3		PBE-D3		TPSS-D3		LC-BOP	M06-L
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}
1	1.9	6.5	−5.3	−0.9	−5.3	−0.6	4.2	8.8	−1.9	−5.1
2	0.0	4.9	−7.7	−3.0	−7.5	−2.4	3.0	7.9	−3.2	−7.0
3	1.1	5.9	−6.1	−1.6	−6.2	−1.2	3.3	8.1	−2.9	−4.6
4	−0.2	4.9	−8.1	−3.2	−7.8	−2.5	2.9	8.0	−3.6	−7.6
5	0.0	5.3	−7.5	−2.4	−7.2	−1.8	3.0	8.2	−3.5	−6.3
6	−0.5	4.7	−8.5	−3.5	−8.1	−2.7	2.8	8.0	−4.3	−8.7
7	0.1	5.2	−7.4	−2.6	−7.1	−1.8	3.3	8.2	−3.9	−6.5
8	9.2	11.1	3.0	4.8	0.2	2.1	4.2	6.0	13.8	−0.1
9	10.1	12.0	4.1	5.9	1.2	3.1	5.0	6.8	13.2	−1.9
10	10.8	12.5	3.8	5.5	0.1	1.8	4.9	6.5	7.8	−1.1
11	11.7	13.4	5.0	6.6	1.5	3.2	5.9	7.4	8.6	−1.2
12	9.4	11.4	3.3	5.2	0.6	2.6	4.3	6.2	13.3	0.1
13	11.3	13.4	5.5	7.4	2.6	4.7	6.1	8.1	14.0	−0.3
14	10.5	12.4	3.8	5.5	0.1	1.8	4.8	6.4	7.3	−0.7
15	12.2	14.1	5.6	7.2	2.3	4.0	6.4	8.0	8.7	−2.1
16	10.6	12.7	5.1	7.1	2.4	4.5	5.7	7.7	13.9	0.6
17	11.5	13.6	5.8	7.7	2.9	4.9	6.4	8.3	13.4	−0.5
18	10.9	12.7	4.2	5.9	0.4	2.2	5.0	6.6	7.1	−0.5
19	11.9	13.8	5.3	7.0	2.1	3.9	6.2	7.9	8.4	−2.8
20	10.6	12.8	5.2	7.2	2.6	4.7	5.8	7.8	13.5	0.4
21	7.6	10.6	−1.2	1.7	−0.5	2.6	7.9	10.7	5.9	1.2
22	6.7	8.8	−1.1	0.9	−2.8	−0.6	4.8	6.8	8.2	3.5
23	7.2	10.7	0.3	3.5	0.7	4.1	7.7	10.8	4.2	1.0
24	6.8	10.0	−0.6	2.4	−0.2	2.9	7.1	9.9	4.6	0.6
25	6.2	9.5	−1.5	1.6	−0.8	2.4	6.7	9.6	6.2	0.3
26	7.1	10.4	−1.6	1.5	−0.8	2.5	7.2	10.1	5.0	1.7
27	6.8	10.2	−1.7	1.4	−0.9	2.4	7.2	10.1	4.9	1.3
28	7.8	11.1	−0.6	2.5	0.3	3.5	8.4	11.3	5.0	1.9

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Table 36 – continued from previous page

	BLYP-D3		BP86-D3		PBE-D3		TPSS-D3		LC-BOP	M06-L
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}
29	6.8	10.5	−0.2	3.2	0.4	4.0	7.4	10.6	3.7	1.1
30	5.6	9.3	−1.4	2.1	−0.6	3.1	6.2	9.5	2.9	−0.3
31	7.0	10.0	−1.2	1.6	−1.8	1.0	6.1	8.7	6.7	1.9
32	6.3	9.9	−2.3	1.1	−1.2	2.3	7.0	10.2	4.9	0.0
33	6.6	10.3	−1.6	1.9	−0.4	3.3	7.3	10.6	2.7	2.0
34	7.9	11.3	−0.3	2.9	0.7	4.0	8.6	11.6	4.4	2.0
35	7.7	11.5	0.7	4.3	1.4	5.0	8.2	11.5	4.1	2.3
36	7.6	11.3	−1.0	2.5	0.3	3.9	8.5	11.7	5.8	1.4
37	7.7	11.5	−0.5	3.0	0.7	4.4	8.4	11.8	3.4	3.0
38	−2.7	4.1	−0.4	6.3	−0.4	6.7	−1.0	6.0	−6.5	−3.7
39	−4.2	3.1	−1.7	5.4	−1.7	5.9	−2.5	4.7	−5.8	−6.1
40	−3.0	4.3	−0.6	6.5	−0.5	7.1	−1.3	6.0	−7.5	−3.0
41	−4.1	3.5	−1.6	5.8	−1.6	6.4	−2.6	5.0	−6.1	−7.0
42	−2.9	4.7	−0.5	6.9	−0.2	7.6	−1.2	6.4	−8.0	−2.9
43	−4.3	3.7	−1.7	6.1	−1.5	6.7	−2.9	5.0	−6.4	−7.0
44	−3.2	4.5	−0.8	6.7	−0.5	7.4	−1.4	6.2	−8.7	−3.3
45	−14.1	−2.5	−9.8	2.0	−10.0	2.4	−9.9	2.4	−12.4	−7.6
46	−15.1	−6.3	−14.1	−5.1	−16.4	−6.8	−15.3	−5.9	−14.7	−6.8
47	−7.0	1.2	−3.1	5.2	−5.3	3.5	−4.5	4.2	−8.3	−3.9
48	−17.2	−4.3	−11.5	1.5	−11.8	2.0	−12.0	1.7	−14.8	−11.3
49	−17.7	−6.7	−15.5	−4.3	−17.7	−6.0	−16.7	−5.1	−16.7	−9.4
50	−8.8	0.2	−4.6	4.4	−6.8	2.8	−6.0	3.4	−9.7	−5.8
51	−13.9	−2.2	−9.6	2.4	−9.9	2.8	−8.8	3.6	−13.9	−6.6
52	−18.7	−4.9	−12.9	1.0	−12.8	1.9	−13.3	1.3	−15.8	−12.5
53	−19.1	−7.4	−16.1	−4.3	−18.2	−5.8	−17.3	−5.0	−17.5	−9.1
54	−9.7	−0.2	−5.1	4.3	−7.2	2.8	−6.7	3.1	−10.6	−5.2
55	−14.0	−1.8	−9.3	3.1	−9.6	3.5	−8.7	4.2	−13.9	−5.5
56	−2.6	2.9	−4.9	0.5	−5.2	0.4	1.4	6.8	−3.8	−2.3
57	−4.9	1.2	−7.6	−1.5	−7.6	−1.3	0.1	6.3	−5.5	−5.5
58	−3.2	2.6	−5.6	0.1	−5.8	0.1	0.8	6.5	−5.2	−3.0
59	−6.1	0.2	−6.9	−0.7	−7.5	−1.0	−0.3	6.0	−6.2	−3.1
60	−3.4	2.5	−5.8	0.1	−5.9	0.1	0.7	6.6	−5.8	−3.2

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Table 36 – continued from previous page

	BLYP-D3		BP86-D3		PBE-D3		TPSS-D3		LC-BOP	M06-L
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}
61	−6.1	0.8	−8.9	−2.1	−8.8	−1.7	−0.8	6.0	−6.8	−7.1
62	−3.6	2.4	−5.9	0.0	−6.0	0.1	0.6	6.5	−6.1	−2.9
63	−3.4	4.7	0.5	8.3	1.3	9.5	−0.8	7.0	−6.8	−3.8
64	−5.5	−2.2	−11.9	−8.8	−12.1	−8.7	−2.9	0.4	−2.9	−8.7
65	−5.8	−2.6	−12.3	−9.3	−12.7	−9.5	−4.1	−1.0	−3.4	−9.0
66	−5.6	−2.1	−11.7	−8.5	−12.0	−8.4	−3.1	0.4	−3.8	−8.8
67	−4.3	−1.1	−9.7	−6.7	−11.0	−7.7	−2.8	0.5	−3.6	−6.8
68	−5.6	−2.2	−11.8	−8.5	−12.3	−8.9	−4.0	−0.7	−3.8	−8.5
69	−6.4	−2.7	−12.6	−9.0	−12.9	−9.0	−3.9	−0.2	−4.9	−10.1
70	−5.2	−1.7	−10.6	−7.3	−11.8	−8.2	−3.5	0.0	−4.5	−7.2
71	−6.2	−2.8	−12.3	−9.0	−12.9	−9.3	−4.6	−1.2	−5.0	−9.0
72	−6.0	−2.3	−12.1	−8.6	−12.4	−8.6	−3.5	0.2	−4.8	−9.5
73	−5.2	−1.6	−10.5	−7.1	−11.8	−8.1	−3.5	0.0	−4.9	−7.0
74	−6.3	−2.7	−12.4	−9.0	−13.0	−9.3	−4.6	−1.1	−5.3	−9.1
75	8.6	10.3	2.3	3.8	−0.7	0.9	2.8	4.3	9.0	−4.8
76	8.2	10.1	2.9	4.6	0.1	1.9	2.6	4.3	7.5	−4.3
77	7.6	9.3	2.3	3.9	−0.7	0.9	2.5	4.0	7.8	−4.6
78	8.8	10.4	2.8	4.3	−0.1	1.4	2.8	4.3	8.2	−3.9
79	8.1	10.1	3.0	4.8	0.1	2.0	2.5	4.3	6.7	−4.8
80	7.9	9.7	3.0	4.6	0.0	1.6	3.1	4.6	7.7	−3.7
81	8.4	10.2	2.6	4.2	−0.4	1.4	2.5	4.1	7.3	−4.4
82	8.8	10.8	3.6	5.5	0.8	2.7	3.2	5.0	7.0	−4.1
83	8.3	10.1	3.3	4.8	0.1	1.8	3.2	4.7	7.5	−3.7
84	9.0	10.9	3.3	5.0	0.3	2.1	3.2	4.9	7.6	−3.6
85	−1.1	0.9	−4.9	−3.1	−6.5	−4.7	−1.1	0.5	3.4	−2.8
86	−0.4	1.8	−5.6	−3.6	−6.2	−4.3	0.3	2.1	4.6	−4.4
87	3.1	5.4	−1.4	0.6	−1.9	0.2	3.4	5.3	0.4	1.7
88	−0.2	2.0	−6.2	−4.3	−6.4	−4.6	0.3	1.9	3.5	−3.8
89	−1.7	0.5	−4.8	−2.9	−6.5	−4.5	−1.6	0.1	2.4	−2.2
90	−0.2	1.8	−4.8	−3.0	−5.8	−4.0	0.4	2.0	3.7	−3.5
91	−1.9	0.6	−5.0	−2.9	−6.7	−4.5	−1.8	0.1	2.4	−2.2
92	−0.1	2.0	−4.7	−2.8	−5.7	−3.9	0.5	2.1	3.8	−3.4

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Table 36 – continued from previous page

	BLYP-D3		BP86-D3		PBE-D3		TPSS-D3		LC-BOP	M06-L
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}
93	−0.6	1.8	−5.4	−3.4	−6.0	−4.0	0.0	1.8	4.0	−3.9
94	−0.4	1.8	−5.3	−3.3	−5.8	−3.9	0.2	1.9	4.0	−3.8
95	−0.1	2.1	−1.9	0.0	−4.0	−2.1	0.5	2.2	2.7	−2.4
96	0.1	2.6	−4.3	−2.2	−5.3	−3.2	0.9	2.7	3.8	−2.6
97	0.2	2.5	−1.8	0.2	−3.7	−1.8	1.0	2.7	2.8	−2.2
98	4.0	6.7	0.1	2.6	−0.7	1.8	3.9	6.1	−0.1	2.9
99	0.0	2.6	−3.1	−0.7	−4.4	−2.1	0.2	2.3	2.7	−3.4
100	0.1	2.6	−4.4	−2.2	−5.1	−2.9	0.9	2.7	4.0	−3.1
101	−0.6	2.1	−3.7	−1.4	−4.3	−2.1	−0.2	1.8	2.4	−3.0
102	0.0	2.4	−4.3	−2.2	−5.3	−3.2	0.8	2.6	3.4	−2.5
103	0.0	2.5	−2.0	0.1	−3.8	−1.8	1.0	2.8	2.7	−2.1
104	0.2	2.5	−4.1	−2.2	−5.1	−3.2	1.0	2.6	3.4	−2.5
105	−0.5	2.3	−5.7	−3.3	−5.8	−3.5	0.0	2.0	1.8	−2.2
106	0.2	2.5	−4.4	−2.4	−5.0	−3.0	0.9	2.7	3.6	−3.1
107	−7.9	−2.6	−6.0	−1.0	−6.7	−1.3	−6.8	−1.6	−6.6	−7.1
108	−6.7	−2.0	−6.9	−2.3	−8.1	−3.3	−7.3	−2.5	−6.8	−6.1
109	−8.4	−2.5	−6.0	−0.4	−6.6	−0.6	−7.4	−1.6	−7.2	−7.7
110	−6.7	−1.2	−4.3	1.0	−5.6	0.0	−6.2	−0.8	−6.8	−6.5
111	−7.0	−1.8	−6.5	−1.5	−7.5	−2.2	−7.5	−2.4	−7.0	−6.4
112	−8.3	−2.4	−5.5	0.2	−6.1	0.0	−7.3	−1.4	−7.7	−8.8
113	−6.9	−1.3	−4.4	1.0	−5.7	0.0	−6.5	−1.0	−7.3	−6.1
114	−7.3	−1.6	−6.3	−0.8	−7.4	−1.7	−7.7	−2.2	−7.7	−6.6
115	−8.2	−2.2	−5.3	0.5	−5.9	0.3	−7.1	−1.2	−7.7	−8.5
116	−7.3	−1.6	−4.5	0.9	−5.9	−0.1	−6.8	−1.3	−8.2	−6.4
117	−7.6	−1.7	−6.4	−0.8	−7.6	−1.6	−7.9	−2.2	−8.1	−6.4
118	−17.1	−9.1	−12.8	−4.7	−14.5	−6.1	−14.6	−6.2	−13.9	−10.1
119	−12.1	−4.6	−6.6	0.9	−8.6	−1.0	−9.7	−2.2	−9.5	−7.0
120	−17.0	−8.8	−13.4	−5.1	−15.6	−7.0	−15.6	−7.1	−15.2	−11.2
121	−12.6	−5.0	−7.2	0.3	−9.2	−1.5	−9.8	−2.2	−9.9	−7.4
122	−16.0	−7.4	−11.6	−3.0	−13.5	−4.5	−13.8	−4.9	−13.7	−10.3
123	−11.7	−4.0	−5.5	2.2	−8.5	−0.6	−10.2	−2.4	−10.7	−6.6
124	−17.7	−9.4	−12.8	−4.4	−14.8	−6.1	−14.7	−6.0	−14.6	−9.0

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Table 36 – continued from previous page

	BLYP-D3		BP86-D3		PBE-D3		TPSS-D3		LC-BOP	M06-L
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}
125	−12.3	−4.6	−5.4	2.2	−8.2	−0.3	−9.0	−1.2	−10.5	−6.8
126	−12.4	−4.5	−6.4	1.3	−8.9	−0.9	−9.6	−1.7	−10.7	−6.9
127	−17.4	−8.5	−12.0	−3.1	−14.1	−4.8	−14.3	−5.1	−14.8	−9.3
128	−9.0	−5.1	−10.5	−6.6	−11.4	−7.4	−5.3	−1.4	−5.8	−6.8
129	−9.2	−5.3	−11.2	−7.2	−12.2	−8.2	−6.2	−2.2	−6.2	−7.0
130	−9.0	−4.7	−9.9	−5.7	−11.0	−6.7	−5.3	−1.1	−6.2	−4.8
131	−7.7	−3.9	−8.4	−4.5	−10.2	−6.3	−4.8	−0.8	−5.7	−5.6
132	−9.1	−5.0	−10.7	−6.6	−11.8	−7.6	−6.2	−2.1	−6.5	−6.6
133	−10.0	−5.5	−11.1	−6.6	−12.1	−7.4	−6.3	−1.8	−7.3	−7.6
134	−8.5	−4.3	−9.1	−4.9	−10.9	−6.6	−5.5	−1.3	−6.6	−5.0
135	−9.8	−5.3	−11.2	−6.8	−12.3	−7.8	−6.8	−2.4	−7.3	−7.1
136	−9.7	−5.2	−10.8	−6.3	−11.7	−7.1	−6.0	−1.5	−7.3	−6.7
137	−8.8	−4.4	−9.2	−4.9	−11.0	−6.6	−5.7	−1.4	−7.2	−4.9
138	−9.8	−5.2	−11.3	−6.7	−12.3	−7.6	−6.7	−2.2	−7.5	−6.9
139	−7.4	−2.0	−4.2	1.1	−4.7	0.8	−5.4	−0.1	−8.1	−4.5
140	−7.9	−1.6	−3.8	2.3	−4.2	2.2	−5.9	0.2	−8.9	−5.4
141	−6.8	−1.0	−3.0	2.5	−4.1	1.7	−5.5	0.1	−9.0	−4.3
142	−2.3	0.8	−6.5	−3.5	−7.5	−4.3	−4.1	−1.0	−3.9	−3.5
143	−1.4	1.5	−5.1	−2.3	−6.6	−3.5	−3.8	−0.8	−3.7	−3.8
144	−0.8	1.8	−4.2	−1.7	−5.6	−2.8	−3.1	−0.3	−1.8	−3.4
145	−3.9	−1.0	−7.8	−5.0	−8.9	−5.8	−4.8	−1.7	−2.9	−4.2
146	−3.0	−0.4	−6.3	−3.8	−7.9	−5.1	−4.3	−1.6	−2.5	−4.7
147	−2.0	0.5	−5.6	−3.1	−6.9	−4.2	−3.5	−0.8	−0.5	−4.1
148	14.4	15.9	8.1	9.5	3.9	5.4	8.3	9.7	11.8	8.8
149	4.5	6.3	−3.1	−1.5	−6.7	−4.9	−2.2	−0.5	11.1	−1.8
150	7.4	10.2	1.1	4.1	−1.5	1.9	2.0	5.3	6.1	2.0
151	4.5	8.6	2.7	6.9	1.2	6.0	4.1	9.0	4.7	−0.1
152	0.7	4.6	−0.5	3.3	−2.6	1.6	−1.4	2.8	2.7	−0.3
153	−2.9	1.9	1.6	6.4	−0.6	4.6	−1.7	3.4	0.7	2.5
154	0.7	5.2	−2.4	2.1	−3.9	1.0	−2.4	2.4	−3.4	0.3
155	−2.4	2.5	−2.1	2.7	−3.9	1.3	−2.5	2.7	−2.3	−2.8
156	−0.6	4.3	0.0	4.8	−0.8	4.3	−1.1	3.9	−2.2	−3.0

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Table 36 – continued from previous page

	BLYP-D3		BP86-D3		PBE-D3		TPSS-D3		LC-BOP	M06-L
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}
157	−3.8	1.9	−3.4	2.4	−5.5	0.6	−3.1	2.9	−4.0	−3.1
158	14.3	15.9	8.2	9.6	4.0	5.5	8.3	9.7	11.0	8.6
159	14.0	15.5	7.9	9.3	3.7	5.2	8.0	9.4	11.0	8.3
160	7.4	10.3	1.3	4.3	−1.3	2.0	2.1	5.4	5.4	1.9
161	7.8	12.2	5.9	10.4	4.2	9.3	7.2	12.4	6.9	1.0
162	1.0	5.1	−0.8	3.4	−3.3	1.2	−1.6	3.0	2.7	2.4
163	−0.9	4.2	1.4	6.5	−0.2	5.3	−0.7	4.8	0.9	−1.0
164	−0.8	4.0	−3.7	1.2	−5.6	−0.4	−4.0	1.1	−3.6	−0.1
165	−2.5	2.3	−4.8	0.1	−6.9	−1.7	−4.4	0.8	−0.6	−0.7
166	−1.7	4.2	−0.6	5.1	−1.8	4.4	−2.4	3.6	−5.7	−3.5
167	−4.5	1.2	−4.3	1.3	−6.3	−0.3	−4.8	1.2	−2.8	−2.8
168	14.5	16.0	8.3	9.8	4.2	5.8	8.4	9.9	10.7	8.7
169	14.4	15.9	8.3	9.7	4.1	5.6	8.3	9.7	11.1	8.5
170	5.6	8.5	−0.3	2.7	−3.0	0.4	0.6	3.9	5.5	0.6
171	3.0	6.7	−1.8	2.1	−4.5	−0.2	−1.3	3.0	4.6	−1.4
172	0.1	4.8	−1.1	3.6	−2.9	2.2	−1.5	3.6	3.9	1.5
173	−3.0	2.2	0.3	5.3	−2.1	3.3	−2.7	2.7	0.6	−1.7
174	−2.4	2.6	−4.7	0.3	−6.8	−1.4	−4.4	1.0	−1.2	−1.1
175	−3.1	3.4	−2.6	3.8	−4.3	2.6	−4.0	2.8	−6.8	−2.9
176	−4.7	1.5	−3.2	3.0	−4.8	1.9	−3.6	3.0	−3.2	−2.7
177	14.8	16.4	8.6	10.1	4.5	6.1	8.8	10.2	10.8	9.0
178	6.2	8.3	0.3	2.3	−2.9	−0.8	0.5	2.4	11.9	−2.6
179	5.8	8.7	−0.1	2.9	−2.8	0.6	0.8	4.1	5.4	0.7
180	6.4	9.3	0.3	3.3	−2.2	1.2	1.1	4.5	3.8	0.9
181	−2.8	3.0	−2.0	3.9	−4.2	2.2	−3.6	2.7	1.4	−0.2
182	−2.8	3.1	−1.7	4.3	−3.8	2.6	−3.4	3.1	1.4	−0.4
183	−0.1	4.9	−3.0	2.1	−4.9	0.5	−3.4	2.0	−3.7	0.3
184	−2.0	3.0	−4.3	0.7	−6.4	−1.0	−4.0	1.4	−1.0	−0.9
185	−2.3	4.3	−2.5	3.8	−4.2	2.7	−3.9	2.8	−6.1	−2.2
186	−3.4	2.6	−3.3	2.6	−5.2	1.2	−3.6	2.7	−2.1	−1.3
187	9.0	10.8	3.6	5.3	0.3	2.1	5.8	7.5	7.2	4.1
188	1.9	5.5	−1.7	2.1	−3.5	0.7	0.1	4.2	4.2	−2.7

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Table 36 – continued from previous page

	BLYP-D3		BP86-D3		PBE-D3		TPSS-D3		LC-BOP	M06-L
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}
189	−6.1	−0.6	−4.6	0.9	−5.9	0.1	−5.0	0.9	2.8	−2.7
190	−8.8	−2.8	−7.4	−1.5	−7.7	−1.4	−6.7	−0.6	−6.5	−4.2
191	−9.6	−3.8	−8.3	−2.5	−8.9	−2.7	−7.0	−0.8	−3.1	−3.6
192	9.1	11.2	4.0	5.9	0.9	3.0	6.1	8.0	6.6	2.6
193	0.8	4.8	−2.8	1.3	−4.7	−0.1	−0.9	3.6	2.4	−3.6
194	−7.9	−1.8	−5.4	0.7	−6.5	0.1	−5.9	0.6	1.2	−3.3
195	−9.9	−3.4	−8.3	−1.9	−8.5	−1.7	−7.8	−1.3	−8.1	−5.9
196	−10.8	−4.8	−8.8	−2.8	−9.4	−3.0	−7.8	−1.6	−4.3	−4.9
197	10.2	12.1	4.3	6.1	2.0	3.9	4.7	6.4	10.2	−3.8
198	2.2	6.0	−0.8	3.1	−2.2	2.1	−0.2	4.1	3.3	−7.7
199	−5.7	0.0	−2.3	3.4	−3.6	2.5	−4.3	1.6	1.8	−5.5
200	−7.6	−1.1	−5.2	1.0	−5.0	1.6	−5.9	0.5	−4.7	−8.9
201	−10.2	−3.5	−7.5	−0.9	−8.3	−1.4	−7.0	−0.3	−3.8	−8.8
202	9.0	10.9	3.6	5.3	0.0	1.8	5.8	7.5	5.6	5.3
203	0.8	4.2	−4.2	−0.7	−6.1	−2.3	−2.0	1.8	2.3	−3.3
204	−4.6	−0.1	−4.7	−0.2	−6.3	−1.5	−4.9	−0.1	1.4	−1.2
205	−6.7	−1.5	−7.4	−2.3	−8.2	−2.8	−6.9	−1.6	−7.4	−4.2
206	−8.2	−3.5	−8.3	−3.6	−9.4	−4.4	−6.8	−1.8	−2.6	−1.7
207	8.4	10.2	2.2	3.8	−0.6	1.1	2.9	4.5	9.6	−4.9
208	2.0	5.4	−1.0	2.4	−2.7	1.0	−0.3	3.4	3.5	−6.3
209	−5.7	−1.3	−3.5	0.9	−4.9	−0.3	−5.1	−0.3	1.0	−5.1
210	−6.7	−1.6	−5.7	−0.9	−6.4	−1.2	−6.7	−1.7	−5.8	−8.2
211	−6.3	−1.6	−4.6	0.0	−5.3	−0.5	−4.5	0.2	−1.5	−5.8
212	9.6	11.2	4.5	5.9	0.5	2.1	6.0	7.5	7.8	7.1
213	3.3	6.2	−1.9	1.1	−4.0	−0.7	−0.5	2.9	5.2	0.0
214	−3.4	1.1	−2.9	1.6	−4.6	0.3	−4.0	0.9	5.1	−0.7
215	−2.5	2.2	−5.4	−0.8	−6.6	−1.6	−5.3	−0.4	−3.6	−2.1
216	−6.5	−1.8	−8.1	−3.4	−9.7	−4.6	−7.1	−2.1	−2.0	−3.2
217	9.7	11.4	4.2	5.8	0.5	2.3	5.8	7.5	8.3	5.1
218	1.1	4.6	−3.9	−0.3	−5.8	−1.8	−2.3	1.6	2.8	−2.5
219	−5.4	−0.4	−4.8	0.3	−6.1	−0.6	−5.5	0.0	3.1	−3.7
220	−6.4	−0.9	−7.2	−1.8	−8.2	−2.4	−7.6	−1.9	−6.4	−5.1

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Table 36 – continued from previous page

	BLYP-D3		BP86-D3		PBE-D3		TPSS-D3		LC-BOP	M06-L
	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}
221	−7.2	−1.8	−7.9	−2.4	−9.8	−4.0	−7.0	−1.2	−3.7	−5.0
222	11.2	12.8	5.8	7.2	3.1	4.7	6.4	7.8	13.9	−3.5
223	1.6	5.2	−3.3	0.4	−5.1	−1.0	−1.9	2.1	1.9	−1.9
224	−6.7	−1.8	−3.4	1.5	−5.1	0.3	−5.1	0.3	1.0	−3.8
225	−3.9	1.4	−4.9	0.4	−6.0	−0.4	−5.7	−0.3	−6.9	−2.8
226	−8.6	−2.8	−8.4	−2.7	−9.0	−2.8	−7.6	−1.5	−4.3	−4.0
227	9.9	11.3	4.8	6.1	0.8	2.2	6.0	7.3	10.9	6.6
228	1.9	4.2	−2.0	0.4	−4.3	−1.6	−1.3	1.5	6.5	−0.4
229	−3.4	0.0	−2.9	0.5	−5.0	−1.1	−4.0	0.0	4.3	0.1
230	−4.0	−0.1	−4.6	−0.7	−6.5	−2.5	−5.3	−1.3	−4.3	−0.7
231	−1.3	2.1	−3.2	0.2	−4.8	−1.1	−2.6	1.1	3.6	0.1
232	10.3	11.7	5.5	6.8	1.6	3.0	6.4	7.8	10.5	6.0
233	3.4	6.6	−0.8	2.5	−2.9	0.7	−0.1	3.5	5.3	−1.5
234	−2.9	1.5	−2.1	2.3	−3.6	1.3	−3.0	1.8	5.7	−1.9
235	−3.8	1.3	−4.6	0.4	−6.0	−0.7	−5.9	−0.7	−4.9	−3.9
236	−5.6	−1.0	−6.9	−2.2	−8.7	−3.8	−6.3	−1.4	−1.3	−3.4
MAXD	−19.1	16.4	−16.1	10.4	−18.2	−9.5	−17.3	12.4	−17.5	−12.5
MD	−1.1	3.3	−3.4	0.8	−4.9	−0.3	−1.5	2.9	−0.4	−3.1
MAD	6.4	5.4	5.1	3.5	5.4	3.2	4.8	4.0	6.1	4.2

Table 37: Deviation of interaction energy ΔE in kJ/mol to the reference values of the IL–2013 set of selected hybrid functionals in combination with the 6–31++G** basis set. E_{NCP}: without counter poise correction; E_{CP}: with counter poise correction; MAXD: maximum deviation; MD: mean deviation; MAD: mean absolute deviation;

	B3LYP-D3		M05-2X	M06	M06-2X	M08-SO	M08-HX
	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}
1	−9.4	−4.9	0.4	1.7	−9.2	−4.4	−6.1
2	−12.2	−7.4	−0.3	−0.3	−10.2	−5.5	−7.2
3	−10.2	−5.6	−0.1	1.0	−9.0	−4.1	−6.0
4	−12.8	−7.9	−0.3	−0.9	−10.4	−5.3	−7.0
5	−11.8	−6.8	−0.1	0.4	−10.1	−5.0	−6.8

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Table 37 – continued from previous page

	B3LYP-D3		M05-2X	M06	M06-2X	M08-SO	M08-HX
	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}
6	−13.3	−8.3	−1.0	−2.1	−11.2	−5.9	−7.7
7	−11.9	−7.1	−0.3	0.5	−10.2	−5.1	−7.0
8	11.4	13.2	9.7	−1.3	5.2	0.2	3.1
9	12.1	13.9	10.7	−2.4	5.0	−0.8	2.2
10	9.9	11.6	11.2	1.7	5.6	5.6	3.5
11	10.8	12.4	11.6	1.5	5.8	4.8	3.4
12	11.5	13.4	9.7	−0.7	5.1	0.0	3.0
13	13.3	15.3	12.0	−0.8	6.3	0.5	3.5
14	9.6	11.4	11.1	2.0	5.7	5.7	3.5
15	11.4	13.2	11.5	0.8	5.0	3.3	2.3
16	13.1	15.1	10.6	−0.1	5.5	0.5	3.4
17	13.4	15.4	11.8	−0.9	6.2	0.3	3.4
18	9.9	11.7	11.2	2.5	5.8	6.1	4.0
19	11.1	12.9	11.2	0.5	4.5	2.7	1.8
20	13.1	15.1	10.6	0.0	5.4	0.2	3.2
21	2.7	5.6	10.0	5.0	−0.4	−1.2	−1.4
22	2.4	4.6	11.1	4.7	5.6	4.7	4.0
23	3.4	6.6	10.0	3.4	0.0	−1.0	−1.2
24	2.5	5.5	10.2	5.1	0.2	−0.5	−1.1
25	2.2	5.3	10.4	3.2	0.3	−1.0	−1.1
26	1.8	4.9	9.9	5.3	0.3	−0.5	−0.5
27	2.0	5.2	9.6	4.5	−0.5	−1.5	−1.3
28	2.8	5.9	9.6	5.2	−0.8	−1.3	−1.6
29	2.9	6.3	10.0	3.5	−0.1	−1.2	−1.3
30	2.1	5.5	10.1	4.5	−1.2	−1.9	−2.7
31	2.1	4.9	10.3	4.0	2.2	1.9	0.9
32	1.2	4.5	10.4	2.8	−0.6	−1.4	−1.4
33	1.8	5.2	9.5	5.9	−1.1	−1.5	−1.8
34	2.9	6.0	9.5	5.2	−0.9	−1.3	−1.7
35	3.7	7.2	11.2	4.8	1.1	0.0	−0.2
36	2.4	5.8	12.0	4.3	0.7	−0.1	−0.1
37	2.7	6.2	10.3	7.1	−0.4	−0.7	−1.2

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Table 37 – continued from previous page

	B3LYP-D3		M05-2X	M06	M06-2X	M08-SO	M08-HX
	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}
38	−2.1	4.6	−1.4	−0.8	−10.9	−10.5	−10.2
39	−2.5	4.6	−1.1	−1.8	−11.6	−11.2	−11.4
40	−2.4	4.7	−1.7	−0.8	−11.0	−10.7	−10.3
41	−2.5	5.0	−1.2	−2.4	−12.1	−12.0	−12.1
42	−2.3	5.0	−1.6	−0.7	−11.0	−10.6	−10.3
43	−2.7	5.1	−0.8	−1.5	−12.0	−11.8	−12.1
44	−2.7	4.7	−2.1	−1.4	−11.4	−11.0	−10.7
45	−12.6	−0.7	−1.7	−3.2	−13.5	−13.0	−15.7
46	−14.3	−5.0	−1.7	−5.0	−6.2	−2.7	−5.2
47	−8.6	−0.2	0.0	−1.1	−8.0	−6.7	−6.8
48	−15.0	−1.8	−2.1	−7.4	−14.9	−14.4	−16.3
49	−17.0	−5.6	−3.1	−7.0	−9.0	−6.0	−8.6
50	−10.3	−1.2	−0.2	−2.7	−9.0	−7.8	−8.2
51	−13.4	−1.4	−2.2	−4.1	−13.7	−12.9	−15.9
52	−16.3	−2.3	−2.0	−7.0	−15.5	−15.4	−17.5
53	−18.1	−6.1	−2.6	−6.9	−9.0	−6.5	−9.2
54	−11.0	−1.5	0.1	−2.2	−8.7	−7.4	−8.1
55	−13.5	−1.1	−1.4	−2.9	−13.2	−12.0	−15.6
56	−10.1	−4.8	1.4	3.1	−7.7	−3.6	−5.7
57	−13.4	−7.3	0.4	−0.2	−9.5	−5.5	−7.4
58	−10.9	−5.2	0.4	2.0	−8.6	−4.4	−6.6
59	−12.9	−6.8	1.5	1.2	−7.8	−4.3	−6.2
60	−11.2	−5.4	0.3	1.8	−8.7	−4.5	−6.7
61	−15.2	−8.5	0.2	−1.6	−10.3	−5.4	−7.2
62	−11.4	−5.6	0.4	2.5	−8.7	−4.4	−6.9
63	−2.7	5.2	−0.7	−0.4	−11.7	−12.4	−11.8
64	−13.8	−10.5	−0.8	−3.1	−8.1	−3.5	−5.4
65	−13.3	−10.2	−1.5	−4.2	−7.9	−3.1	−4.9
66	−14.0	−10.6	−1.0	−3.2	−8.2	−3.2	−4.9
67	−11.7	−8.6	0.1	−2.1	−5.8	−2.2	−3.4
68	−13.0	−9.7	−1.1	−3.9	−7.3	−2.5	−4.1
69	−15.1	−11.4	−1.6	−4.2	−9.0	−3.9	−5.3

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Table 37 – continued from previous page

	B3LYP-D3		M05-2X	M06	M06-2X	M08-SO	M08-HX
	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}
70	−12.6	−9.2	−0.6	−2.5	−6.5	−2.6	−4.1
71	−13.8	−10.4	−1.2	−4.1	−7.5	−2.7	−4.0
72	−14.8	−11.1	−1.4	−3.9	−8.6	−3.2	−4.8
73	−12.7	−9.2	−0.4	−2.2	−6.2	−2.4	−3.8
74	−14.0	−10.5	−1.4	−4.3	−7.6	−2.7	−4.2
75	9.0	10.6	9.8	−0.4	3.9	−1.5	−1.1
76	9.0	10.7	9.0	−0.4	3.3	−2.3	−1.0
77	8.7	10.3	10.1	−0.7	3.9	−0.6	−0.3
78	9.1	10.7	9.8	0.6	4.2	−1.3	−0.6
79	8.9	10.8	8.8	−1.0	2.9	−2.5	−1.0
80	9.2	10.8	10.3	−0.1	4.2	−0.3	0.1
81	8.7	10.4	9.4	0.2	3.8	−1.6	−0.8
82	9.5	11.4	9.3	−0.4	3.5	−1.9	−0.5
83	9.4	11.0	10.6	0.2	4.5	0.0	0.6
84	9.3	11.1	9.9	0.8	4.4	−0.9	−0.2
85	−1.7	0.1	7.3	−0.2	1.6	−0.4	0.3
86	−2.2	−0.1	7.2	0.2	0.1	−1.5	−1.9
87	−0.8	1.3	5.6	2.6	−1.9	−1.9	−3.4
88	−2.8	−0.8	6.7	0.2	0.2	−1.3	−1.4
89	−2.0	0.0	7.1	0.4	1.7	−0.3	0.7
90	−1.9	0.0	7.4	−0.5	1.2	−0.7	−0.4
91	−2.1	0.1	7.1	0.4	1.7	−0.3	0.6
92	−1.8	0.1	7.5	−0.4	1.4	−0.5	−0.2
93	−2.2	−0.1	7.3	1.1	0.3	−1.4	−1.5
94	−2.1	−0.1	7.3	0.9	0.4	−1.3	−1.5
95	0.3	2.3	7.8	−1.3	2.2	0.3	1.5
96	−1.5	0.6	7.9	0.1	1.8	−0.1	0.2
97	0.2	2.3	7.8	−1.4	2.1	0.2	1.4
98	0.2	2.6	6.1	4.2	−0.8	−0.7	−2.3
99	−0.5	1.9	7.6	0.2	1.2	−0.5	0.0
100	−1.5	0.8	8.0	1.8	1.1	−0.4	−0.6
101	−1.4	0.9	7.4	2.5	1.2	0.3	0.8

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Table 37 – continued from previous page

	B3LYP-D3		M05-2X	M06	M06-2X	M08-SO	M08-HX
	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}
102	−1.7	0.5	7.9	0.2	1.9	0.0	0.4
103	0.0	2.2	7.8	−1.2	1.9	0.0	0.9
104	−1.5	0.5	7.9	0.2	2.0	0.0	0.4
105	−2.8	−0.4	7.3	2.0	1.1	−0.6	−0.3
106	−1.6	0.6	7.9	1.7	1.0	−0.5	−0.7
107	−6.1	−0.9	−1.6	−5.3	−8.5	−7.6	−8.1
108	−6.2	−1.4	−0.3	−5.4	−5.5	−4.6	−4.9
109	−6.4	−0.6	−1.9	−5.1	−8.9	−8.2	−8.6
110	−4.7	0.7	−1.1	−4.6	−7.3	−6.8	−7.5
111	−6.1	−1.0	−0.7	−5.3	−6.0	−4.9	−5.1
112	−6.3	−0.4	−2.1	−5.5	−9.3	−8.5	−8.5
113	−4.9	0.6	−1.1	−4.2	−7.2	−6.7	−7.5
114	−6.2	−0.6	−0.4	−5.0	−5.8	−4.6	−4.6
115	−6.2	−0.3	−1.9	−5.3	−9.0	−8.1	−7.9
116	−5.3	0.3	−1.4	−4.3	−7.5	−6.8	−7.6
117	−6.4	−0.7	−0.4	−5.1	−5.8	−4.4	−4.5
118	−14.4	−6.2	−3.4	−6.5	−9.6	−8.3	−10.4
119	−9.9	−2.5	−0.8	−3.5	−6.6	−5.9	−5.7
120	−14.4	−5.9	−3.7	−9.0	−9.0	−7.8	−8.6
121	−10.3	−2.8	−1.7	−4.4	−8.0	−8.0	−8.8
122	−13.8	−5.1	−3.0	−5.2	−9.7	−8.2	−9.7
123	−9.8	−2.1	−0.3	−2.0	−5.7	−4.6	−3.6
124	−15.0	−6.5	−3.1	−6.6	−8.5	−7.1	−8.9
125	−9.7	−2.0	−0.2	−3.9	−6.4	−5.8	−5.9
126	−10.4	−2.6	−1.2	−3.6	−7.1	−6.9	−7.2
127	−14.8	−5.8	−3.0	−5.0	−9.5	−8.2	−10.4
128	−13.8	−9.9	−0.9	−2.3	−7.3	−3.8	−5.5
129	−13.7	−9.7	−1.7	−3.4	−7.3	−3.5	−5.5
130	−13.4	−9.2	0.3	−1.1	−5.8	−2.2	−3.5
131	−11.9	−8.0	−0.2	−1.8	−5.4	−2.6	−4.0
132	−13.5	−9.4	−1.1	−2.9	−6.8	−2.8	−4.7
133	−15.0	−10.5	−1.0	−3.1	−7.7	−3.3	−4.7

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Table 37 – continued from previous page

	B3LYP-D3		M05-2X	M06	M06-2X	M08-SO	M08-HX
	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}
134	−12.6	−8.5	−0.3	−1.7	−5.3	−2.5	−3.8
135	−14.2	−9.8	−1.1	−3.4	−6.9	−2.7	−4.4
136	−14.8	−10.3	−0.6	−2.8	−7.1	−2.9	−4.2
137	−13.0	−8.7	−0.1	−1.4	−5.2	−2.3	−3.6
138	−14.4	−9.8	−1.0	−3.3	−6.9	−2.6	−4.3
139	−6.6	−1.2	−2.0	−5.0	−8.4	−8.4	−8.4
140	−6.9	−0.6	−1.8	−4.6	−8.5	−8.3	−7.8
141	−5.8	−0.1	−1.9	−4.4	−7.6	−7.8	−8.2
142	−4.2	−1.2	2.2	4.1	−3.2	5.7	1.7
143	−3.4	−0.6	0.9	2.6	−3.9	5.4	1.1
144	−2.6	−0.1	1.9	3.4	−3.1	5.7	1.2
145	−4.5	−1.6	3.8	4.1	−1.9	6.9	2.7
146	−3.5	−1.0	2.7	2.5	−2.6	6.8	2.2
147	−2.7	−0.2	4.0	3.9	−1.6	7.1	2.3
148	13.5	15.0	13.8	10.1	9.4	13.0	9.6
149	6.8	8.5	5.5	−4.7	3.3	1.0	3.6
150	4.9	7.8	8.6	9.5	2.5	11.2	5.8
151	5.2	9.3	6.5	4.5	−2.0	0.4	−1.2
152	1.7	5.7	8.2	3.9	3.0	5.3	3.8
153	2.4	7.1	5.7	2.2	−0.4	0.3	0.3
154	−1.9	2.7	1.7	1.8	−2.5	3.5	0.9
155	−2.4	2.6	3.1	1.3	−2.8	−1.5	−2.4
156	−0.3	4.5	−0.4	−0.9	−6.8	−6.6	−5.7
157	−5.2	0.5	0.3	0.5	−6.4	−4.8	−6.1
158	13.3	14.8	13.2	9.6	9.0	12.5	9.2
159	13.1	14.6	13.2	9.5	8.9	12.4	9.1
160	4.8	7.7	8.3	9.3	2.3	11.0	5.6
161	7.4	11.7	7.1	7.3	−2.2	1.2	−1.4
162	1.5	5.8	7.7	7.3	2.6	9.0	5.0
163	1.8	6.9	4.2	4.3	−3.8	−2.1	−3.6
164	−3.0	1.9	0.2	2.6	−3.8	3.5	−0.8
165	−3.0	2.0	4.7	4.5	−0.2	6.9	2.7

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Table 37 – continued from previous page

	B3LYP-D3		M05-2X	M06	M06-2X	M08-SO	M08-HX
	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}
166	−1.6	4.2	−1.7	−2.1	−8.1	−7.8	−7.3
167	−3.8	2.0	3.3	1.1	−2.6	0.7	−0.7
168	13.3	14.8	13.2	9.7	9.0	12.5	9.2
169	13.4	14.9	13.5	9.8	9.2	12.6	9.4
170	3.6	6.5	7.3	8.7	1.5	10.8	4.7
171	3.4	7.2	9.2	7.3	2.5	9.5	5.9
172	1.7	6.6	9.3	6.9	3.3	8.8	5.8
173	0.8	5.9	5.4	1.2	−1.9	−0.8	−1.1
174	−2.9	2.2	4.2	3.8	−0.6	6.8	2.8
175	−3.2	3.3	0.2	−1.8	−5.7	−2.9	−4.0
176	−2.4	4.0	3.5	0.6	−3.7	−0.5	−2.2
177	13.6	15.1	13.5	10.1	9.2	12.8	9.5
178	9.4	11.4	8.9	−3.8	4.9	0.4	3.4
179	3.7	6.6	7.4	8.9	1.6	10.8	4.7
180	3.6	6.6	7.2	8.2	1.2	9.9	4.5
181	0.2	6.2	8.4	5.0	1.6	6.3	3.5
182	0.4	6.4	8.2	4.4	1.0	5.2	2.7
183	−2.6	2.6	0.4	3.2	−3.7	3.7	−0.7
184	−2.6	2.5	4.5	4.1	−0.4	7.0	3.1
185	−2.9	3.6	1.2	−0.3	−4.4	−0.3	−1.7
186	−2.1	4.0	5.1	2.9	−1.0	4.2	1.8
187	10.3	12.1	10.5	4.3	4.4	8.5	6.2
188	2.2	5.8	9.0	6.6	−0.3	9.4	4.8
189	−1.2	4.4	9.2	4.6	0.2	7.7	3.8
190	−6.5	−0.5	1.2	−0.9	−6.6	1.5	−1.4
191	−5.8	0.3	5.0	2.1	−3.2	5.4	1.6
192	10.7	12.7	10.6	2.5	3.8	7.9	5.6
193	0.7	4.7	8.1	4.8	−0.9	8.3	4.0
194	−2.3	3.9	9.0	3.2	−0.3	7.6	3.8
195	−7.6	−1.1	0.2	−2.5	−7.6	0.3	−2.6
196	−6.2	0.0	5.0	1.1	−3.2	5.3	1.6
197	10.2	12.0	10.0	1.4	2.7	−2.2	−1.4

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Table 37 – continued from previous page

	B3LYP-D3		M05-2X	M06	M06-2X	M08-SO	M08-HX
	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}
198	0.5	4.3	3.6	1.5	−6.0	−4.7	−6.3
199	−1.9	3.8	4.9	1.1	−4.9	−2.8	−5.2
200	−6.1	0.2	−2.1	−5.0	−11.4	−10.6	−11.0
201	−9.0	−2.4	0.8	−2.3	−8.7	−7.2	−8.8
202	10.1	11.8	9.7	3.2	3.5	9.2	6.6
203	0.5	3.9	6.9	5.8	−1.1	9.0	4.1
204	−1.0	3.5	8.1	5.8	0.7	9.3	5.5
205	−6.0	−0.8	−0.4	−0.3	−6.6	1.9	−1.2
206	−5.1	−0.2	5.3	3.8	−1.0	8.1	4.3
207	9.1	10.8	10.9	−0.2	3.8	−0.6	−0.8
208	0.6	3.8	3.1	1.1	−5.4	−4.1	−6.4
209	−1.9	2.6	4.3	−1.1	−3.9	−2.1	−4.6
210	−5.7	−0.6	−2.6	−5.9	−9.7	−9.0	−9.9
211	−4.3	0.5	1.1	−0.1	−6.9	−4.4	−6.7
212	10.5	12.0	11.1	6.3	5.6	10.6	7.6
213	3.0	6.0	8.6	9.3	1.8	11.7	6.4
214	1.3	6.0	9.9	6.3	2.4	8.6	5.1
215	−3.7	1.1	1.2	1.1	−3.6	1.4	−0.6
216	−5.7	−0.9	3.7	4.2	−2.1	5.2	1.7
217	10.5	12.2	11.9	6.0	5.9	10.0	7.1
218	0.9	4.4	7.2	6.9	−0.3	9.4	4.1
219	−0.9	4.2	8.1	5.3	−0.8	6.3	2.0
220	−5.9	−0.4	0.1	0.3	−6.1	1.5	−1.5
221	−6.8	−1.2	3.6	2.2	−3.3	3.4	−0.1
222	11.9	13.4	10.9	1.2	2.8	−1.4	−1.4
223	1.1	4.7	7.0	7.1	−0.2	9.4	4.2
224	−2.6	2.4	5.2	−0.1	−3.9	−1.0	−3.6
225	−4.4	1.0	0.0	1.9	−5.2	2.4	−0.5
226	−6.0	−0.1	4.0	2.4	−3.5	4.9	1.2
227	10.9	12.3	13.1	7.9	7.5	11.2	7.9
228	2.5	4.9	9.1	7.9	3.5	8.8	5.8
229	0.3	3.9	9.0	6.5	2.7	9.8	6.0

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Table 37 – continued from previous page

	B3LYP-D3		M05-2X	M06	M06-2X	M08-SO	M08-HX
	E_{NCP}	E_{CP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}	E_{NCP}
230	−4.4	−0.4	0.1	1.4	−3.8	3.5	0.1
231	0.6	4.2	7.2	7.3	2.6	9.0	6.2
232	11.0	12.4	13.1	7.4	7.4	10.4	7.4
233	3.1	6.3	9.0	7.4	1.1	9.6	4.4
234	1.1	5.7	9.2	6.0	0.8	7.7	3.5
235	−4.0	1.1	0.9	−1.0	−4.9	−0.3	−2.5
236	−5.0	−0.2	3.8	3.5	−1.4	5.8	2.2
MAXD	−18.1	15.4	13.8	10.1	−15.5	−15.4	−17.5
MD	−2.1	2.2	4.5	0.8	−2.6	−0.3	−1.8
MAD	6.8	5.6	5.3	3.4	5.1	4.9	4.5