Supplementary material to "Cooperativity in Noncovalent Interactions of Biologically Relevant Molecules"

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Contents

- Fig. S2: Structure of complex 12 (CCC S/S1) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.
- Fig. S3: Structure of complex 24 (CGCplus HB/S2) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.
- Fig. S4: Structure of complex 52 (mCmCmC HB/HB1) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.
- Fig. S5: Structure of complex 55 (mCmCmC HB/T1) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.
- Fig. S6 Structure of complex 61 (mCmCmC S/T5) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.
- Fig. S7: Structure of complex 140 (UUU S/T4) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.
- Table SX: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 12 (CCC S/S1).
- Table SXI: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 24 (CGCplus HB/S2).
- Table SXII: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 52 (mCmCmC HB/HB1).
- Table SXII: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 55 (mCmCmC HB/T1).
- Table SXIV: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 61 (mCmCmC S/T5).
- Table SXV: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 140 (UUU S/T4).

TABLE SI: MP2/TZV(2df,2pd) interaction energies (ΔE), two- (ΔE_{12}, ΔE_{23}, ΔE_{13}), and three-body terms (ΔE_3) in kcal mol^{-1} for DNA base trimers.

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
CCC (14)										
1	-52.86	-26.96	-27.36	1.18	0.29	-48.73	-24.92	-25.30	1.21	0.27
2	-52.27	-26.35	-26.68	0.85	-0.09	-48.26	-24.43	-24.67	0.84	-0.01
3	-50.30	-7.58	-11.85	-26.10	-4.77	-46.39	-6.63	-10.80	-24.17	-4.80
4	-50.20	-27.35	-24.25	1.04	0.36	-46.29	-25.25	-22.45	1.05	0.36
5	-46.32	-23.99	-8.42	-11.21	-2.70	-42.76	-22.21	-7.69	-10.14	-2.71
6	-38.82	-27.26	-11.88	0.42	-0.10	-35.65	-25.12	-10.91	0.44	-0.06
7	-51.39	-24.24	-11.66	-14.56	-0.93	-44.37	-22.16	-9.76	-11.54	-0.91
8	-49.96	-14.62	-8.37	-27.57	0.59	-43.09	-11.27	-7.00	-25.49	0.68
9	-49.08	-25.95	-18.97	-4.87	0.71	-42.61	-23.89	-15.39	-4.10	0.77
10	-47.21	-0.72	-26.90	-20.17	0.58	-41.53	-0.59	-24.93	-16.66	0.65
11	-47.73	-23.17	-9.00	-11.94	-3.62	-43.26	-21.12	-7.88	-10.61	-3.65
12	-36.08	-0.48	-19.53	-16.47	0.40	-29.44	-0.46	-16.23	-13.34	0.59
13	-50.28	-8.45	-16.58	-24.67	-0.59	-43.93	-7.55	-13.21	-22.47	-0.71
14	-41.49	-11.72	-12.73	-11.86	-5.18	-35.90	-9.91	-11.08	-9.86	-5.05
CGCplus (13)										
15	-85.59	2.51	-32.79	-51.29	-4.01	-81.13	2.49	-30.54	-49.09	-4.00
16	-81.59	0.87	-35.88	-51.27	4.69	-77.85	0.91	-34.52	-48.97	4.73
17	-86.17	-33.07	-46.50	0.19	-6.79	-81.64	-30.78	-44.50	0.45	-6.81
18	-79.87	0.24	-33.33	-51.22	4.44	-76.25	0.28	-32.09	-48.91	4.47
19	-78.87	1.34	-34.16	-51.21	5.15	-75.32	1.47	-32.91	-48.97	5.09
20	-77.93	2.57	-34.01	-51.31	4.83	-74.48	2.67	-32.86	-49.07	4.79
21	-80.80	1.18	-47.53	-39.51	5.07	-77.08	1.24	-45.77	-37.66	5.11
22	-75.84	0.48	-41.72	-39.36	4.75	-72.40	0.53	-40.23	-37.48	4.78
23	-79.41	-8.94	-25.61	-50.91	6.05	-71.58	-5.53	-23.49	-48.52	5.96
24	-71.37	-20.02	1.52	-53.13	0.26	-64.81	-16.26	1.55	-50.36	0.27

TABLE SI: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
25	-73.18	-5.01	-32.55	-40.88	5.27	-69.47	-4.06	-31.47	-39.18	5.25
26	-80.09	-9.56	-26.18	-50.47	6.12	-72.37	-6.45	-23.79	-48.13	6.01
27	-75.04	-20.57	-18.48	-39.89	3.90	-68.04	-18.46	-15.36	-38.05	3.82
GGG (12)										
28	-62.38	-17.67	-17.67	-17.67	-9.36	-58.59	-16.47	-16.47	-16.47	-9.17
29	-45.86	-22.40	-22.09	0.08	-1.45	-42.46	-20.66	-20.50	0.09	-1.39
30	-55.05	-1.05	-31.15	-22.67	-0.17	-50.15	-1.07	-28.48	-20.46	-0.14
31	-53.53	-15.62	-19.90	-12.20	-5.81	-48.66	-14.36	-17.57	-10.96	-5.76
32	-53.16	-20.47	-29.26	-2.44	-0.99	-48.29	-18.63	-26.78	-1.82	-1.06
33	-50.41	-12.59	-7.43	-29.03	-1.36	-45.97	-11.31	-6.32	-26.93	-1.42
34	-45.62	-13.64	-0.49	-31.04	-0.45	-41.69	-12.57	-0.49	-28.26	-0.38
35	-43.16	-0.92	-23.97	-17.77	-0.49	-32.78	-0.92	-18.96	-13.06	0.16
36	-62.39	-29.85	-18.07	-15.07	0.60	-52.61	-26.95	-13.92	-12.31	0.57
37	-58.88	-18.80	-14.85	-20.18	-5.06	-51.57	-16.97	-13.62	-16.06	-4.92
38	-58.16	-24.87	-16.95	-14.42	-1.92	-50.34	-21.92	-14.81	-11.68	-1.93
39	-61.05	-17.48	-17.48	-17.48	-8.61	-55.36	-15.64	-15.64	-15.64	-8.44
mAmUmU (12)										
40	-35.02	-17.72	0.60	-18.06	0.16	-31.41	-15.88	0.62	-16.28	0.14
41	-35.02	-17.72	0.60	-18.06	0.16	-31.41	-15.88	0.62	-16.28	0.14
42	-35.53	-6.26	-11.79	-17.68	0.20	-29.08	-4.86	-8.62	-15.94	0.34
43	-37.45	-19.15	-0.89	-17.29	-0.12	-29.07	-15.01	-0.90	-13.59	0.43
44	-33.76	-0.39	-14.13	-19.01	-0.23	-26.18	-0.37	-11.19	-14.82	0.20
45	-43.88	-17.86	-10.24	-15.67	-0.12	-36.25	-13.98	-8.38	-13.84	-0.05
46	-43.33	-17.13	-9.88	-16.33	0.01	-35.80	-13.27	-8.10	-14.49	0.06
47	-42.92	-15.95	-8.93	-17.99	-0.04	-35.29	-14.10	-7.20	-13.98	-0.01
48	-43.26	-17.86	-9.24	-16.28	0.12	-35.72	-13.89	-7.54	-14.45	0.16
49	-43.57	-17.96	-12.61	-12.92	-0.08	-35.59	-14.05	-10.80	-10.71	-0.04

TABLE SI: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
50	-37.49	-17.81	-4.55	-15.08	-0.06	-31.03	-15.97	-3.86	-11.19	-0.01
51	-35.67	-4.94	-13.75	-17.02	0.04	-29.90	-3.99	-10.75	-15.23	0.08
mCmCmC (12)										
52	-33.81	-6.69	0.31	-27.76	0.32	-30.63	-5.88	0.34	-25.45	0.36
53	-52.05	-17.65	-7.46	-27.52	0.58	-43.96	-13.63	-5.87	-25.15	0.69
54	-51.99	-27.43	-7.19	-17.75	0.39	-44.05	-25.14	-5.73	-13.71	0.54
55	-22.14	-0.83	-7.73	-13.59	0.02	-18.48	-0.71	-6.58	-11.27	0.08
56	-40.43	-0.86	-19.79	-19.90	0.12	-31.39	-0.82	-15.60	-15.64	0.66
57	-54.27	-26.10	-15.90	-11.91	-0.37	-46.22	-23.79	-11.78	-10.35	-0.30
58	-52.41	-19.10	-25.99	-8.03	0.71	-44.19	-14.82	-23.54	-6.56	0.74
59	-43.82	-14.85	-14.29	-13.18	-1.50	-37.29	-11.24	-12.86	-11.70	-1.50
60	-44.40	-12.30	-15.10	-15.48	-1.52	-36.13	-10.76	-12.15	-11.96	-1.26
61	-44.93	-15.79	-18.51	-10.24	-0.39	-36.66	-13.32	-14.91	-8.26	-0.17
62	-35.82	-14.68	-11.97	-10.27	1.11	-29.80	-11.24	-10.31	-9.34	1.09
63	-47.07	-15.53	-12.92	-14.00	-4.62	-39.90	-13.13	-10.79	-11.56	-4.42
mTmUmU (12)										
64	-24.65	-0.08	-10.57	-13.80	-0.19	-21.90	-0.07	-9.31	-12.33	-0.18
65	-24.02	-13.79	-9.86	-0.16	-0.20	-21.31	-12.32	-8.64	-0.15	-0.20
66	-32.64	-13.30	-13.57	-5.53	-0.24	-26.05	-9.75	-12.07	-4.15	-0.07
67	-27.45	-13.82	-7.91	-5.46	-0.25	-23.69	-12.32	-6.49	-4.68	-0.21
68	-30.24	-0.13	-14.01	-16.08	-0.02	-23.39	-0.12	-10.99	-12.56	0.29
69	-29.12	-15.58	0.09	-13.54	-0.08	-22.01	-12.24	0.10	-10.09	0.23
70	-39.75	-13.50	-12.04	-14.29	0.08	-32.49	-10.39	-9.68	-12.54	0.13
71	-39.64	-14.19	-13.22	-12.30	0.07	-32.44	-12.48	-10.24	-9.85	0.12
72	-35.95	-6.30	-13.94	-15.42	-0.30	-29.35	-4.98	-12.13	-11.98	-0.26
73	-34.21	-13.24	-13.59	-7.15	-0.23	-27.44	-9.88	-11.95	-5.46	-0.15
74	-29.73	-13.70	-11.74	-4.24	-0.06	-24.10	-12.08	-8.53	-3.52	0.04

TABLE SI: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
75	-38.71	-13.69	-11.14	-13.98	0.10	-31.45	-10.50	-8.80	-12.29	0.15
mUmUmU (12)										
76	-25.05	-13.47	-4.86	-6.55	-0.17	-22.16	-12.07	-4.29	-5.63	-0.17
77	-24.41	-13.56	-10.52	-0.09	-0.24	-21.70	-12.13	-9.30	-0.09	-0.17
78	-18.61	-10.52	0.10	-8.16	-0.03	-16.30	-9.28	0.11	-7.10	-0.04
79	-34.99	-9.80	-13.89	-11.51	0.21	-28.59	-7.63	-12.35	-8.89	0.29
80	-34.09	-7.69	-13.62	-12.85	0.07	-27.66	-5.83	-12.18	-9.81	0.16
81	-32.14	-13.29	-13.44	-5.28	-0.14	-26.81	-10.09	-11.89	-4.72	-0.11
82	-31.04	-13.28	-4.62	-13.05	-0.10	-25.74	-10.09	-4.08	-11.51	-0.06
83	-24.01	0.43	-12.13	-12.12	-0.19	-17.81	0.43	-9.17	-9.18	0.11
84	-38.22	-13.34	-11.20	-13.78	0.09	-31.11	-10.28	-8.84	-12.13	0.14
85	-31.73	-14.60	-4.66	-12.40	-0.06	-26.10	-12.95	-3.87	-9.30	0.02
86	-39.35	-12.12	-14.08	-13.23	0.08	-32.22	-9.73	-12.37	-10.25	0.13
87	-33.89	-14.00	-14.47	-5.06	-0.35	-28.18	-12.14	-11.51	-4.19	-0.33
TAT (12)										
88	-41.50	-21.26	-0.69	-19.54	0.00	-38.04	-19.59	-0.68	-17.80	0.03
89	-38.50	-13.69	-3.18	-21.51	-0.13	-35.07	-12.14	-2.80	-19.98	-0.15
90	-40.66	-0.50	-17.45	-22.22	-0.49	-37.37	-0.52	-15.89	-20.48	-0.47
91	-34.62	0.67	-18.09	-17.39	0.20	-31.12	0.70	-16.36	-15.62	0.16
92	-38.99	-10.22	-10.67	-18.44	0.35	-33.22	-8.91	-7.89	-16.84	0.41
93	-33.33	-0.63	-16.46	-15.96	-0.27	-25.41	-0.64	-12.64	-12.38	0.25
94	-30.71	-14.78	-15.18	-0.53	-0.22	-23.56	-11.54	-11.69	-0.49	0.15
95	-43.28	-17.00	-14.49	-12.20	0.41	-36.24	-15.33	-11.05	-10.29	0.43
96	-42.98	-16.64	-12.09	-14.67	0.42	-35.95	-15.02	-10.19	-11.18	0.45
97	-41.08	-10.06	-13.41	-17.82	0.21	-34.73	-8.69	-10.12	-16.18	0.26
98	-40.21	-8.12	-13.93	-18.43	0.27	-33.41	-6.18	-10.77	-16.78	0.32
99	-40.28	-18.71	-12.88	-8.75	0.05	-33.95	-16.89	-10.57	-6.54	0.05

TABLE SI: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
UUA (16)										
100	-41.25	-21.01	-0.71	-19.53	0.01	-37.83	-19.37	-0.70	-17.78	0.03
101	-39.99	-17.61	-21.53	-0.79	-0.06	-36.74	-16.01	-19.90	-0.79	-0.04
102	-40.45	0.05	-21.88	-18.16	-0.47	-37.00	0.05	-20.20	-16.38	-0.46
103	-40.42	-0.46	-17.43	-22.09	-0.44	-37.18	-0.48	-15.90	-20.38	-0.42
104	-39.52	-21.15	-0.67	-17.74	0.04	-36.02	-19.50	-0.64	-15.95	0.06
105	-38.92	-17.31	-18.86	-3.00	0.25	-35.29	-15.62	-17.25	-2.64	0.23
106	-34.67	-17.53	-18.08	0.72	0.22	-31.10	-15.72	-16.33	0.77	0.17
107	-34.68	-17.48	-18.01	0.62	0.19	-31.09	-15.68	-16.22	0.66	0.16
108	-32.55	-18.50	-10.59	-3.14	-0.32	-29.17	-16.74	-9.32	-2.73	-0.38
109	-30.98	-17.94	-2.53	-9.91	-0.59	-27.66	-16.17	-2.20	-8.64	-0.65
110	-35.66	-7.59	-19.31	-9.21	0.45	-30.39	-5.01	-17.71	-8.12	0.45
111	-29.41	-0.41	-14.82	-13.95	-0.23	-22.43	-0.41	-11.41	-10.85	0.24
112	-26.98	-12.27	-0.18	-14.25	-0.28	-20.46	-9.49	-0.16	-10.86	0.05
113	-42.30	-17.21	-11.54	-13.97	0.41	-35.63	-15.57	-9.77	-10.75	0.46
114	-41.84	-16.37	-14.22	-11.69	0.44	-35.12	-14.79	-10.92	-9.89	0.48
115	-39.22	-4.78	-13.83	-20.78	0.17	-33.17	-3.55	-10.81	-19.12	0.32
UUT (12)										
116	-39.54	-17.61	-0.86	-20.99	-0.08	-36.28	-16.00	-0.86	-19.35	-0.06
117	-39.42	-0.89	-17.51	-20.99	-0.04	-36.19	-0.90	-15.93	-19.34	-0.02
118	-38.84	-3.54	-13.86	-21.42	-0.03	-35.38	-3.11	-12.34	-19.84	-0.09
119	-38.74	-21.30	-3.63	-13.77	-0.04	-35.32	-19.74	-3.21	-12.29	-0.09
120	-34.62	-13.87	0.33	-21.06	-0.03	-31.75	-12.61	0.34	-19.43	-0.05
121	-23.70	0.50	-12.04	-11.91	-0.25	-17.85	0.50	-9.24	-9.13	0.02
122	-23.32	-11.36	-12.19	0.51	-0.29	-17.60	-8.86	-9.31	0.52	0.05
123	-38.16	-11.35	-16.61	-10.57	0.38	-31.89	-9.62	-14.71	-8.04	0.48
124	-36.58	-9.18	-16.01	-11.75	0.36	-30.58	-6.88	-14.27	-9.94	0.52

TABLE SI: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
125	-27.12	-9.33	-5.95	-11.49	-0.35	-21.32	-6.79	-3.99	-10.26	-0.28
126	-38.65	-12.66	-12.83	-12.76	-0.40	-33.28	-10.92	-11.03	-10.97	-0.37
127	-34.00	-7.58	-15.68	-11.03	0.28	-29.02	-6.64	-13.84	-8.86	0.32
UUU (14)										
128	-39.39	-20.88	-0.89	-17.58	-0.04	-36.15	-19.25	-0.90	-15.98	-0.02
129	-38.54	-13.63	-21.27	-3.56	-0.08	-35.13	-12.14	-19.72	-3.13	-0.13
130	-34.42	0.34	-20.92	-13.85	0.01	-31.57	0.34	-19.31	-12.59	-0.01
131	-30.73	-16.68	0.02	-13.94	-0.14	-27.98	-15.18	0.03	-12.67	-0.15
132	-32.24	-17.69	-0.41	-13.88	-0.26	-29.37	-16.10	-0.40	-12.64	-0.23
133	-35.36	-7.09	-20.59	-7.97	0.30	-29.79	-5.86	-18.98	-5.24	0.29
134	-26.86	-14.67	-9.36	-2.40	-0.43	-23.12	-13.14	-8.00	-1.55	-0.43
135	-25.64	-13.97	-9.43	-1.90	-0.35	-22.24	-12.37	-8.44	-1.22	-0.21
136	-22.77	-10.31	-12.05	-0.29	-0.12	-17.16	-7.54	-9.46	-0.30	0.14
137	-36.52	-16.75	-9.11	-11.19	0.53	-30.44	-14.91	-6.66	-9.38	0.51
138	-34.93	-5.02	-20.28	-9.79	0.15	-29.48	-4.17	-18.48	-6.98	0.15
139	-33.80	-19.01	-11.24	-3.99	0.44	-27.94	-17.04	-8.38	-2.90	0.38
140	-34.82	-7.64	-8.38	-19.03	0.24	-29.68	-5.05	-7.44	-17.56	0.37
141	-38.67	-12.75	-12.75	-12.75	-0.42	-33.36	-10.99	-10.99	-10.99	-0.40

TABLE SII: SCS-MP2/TZV(2df,2pd) interaction energies (ΔE), two- (ΔE_{12}, ΔE_{23}, ΔE_{13}), and three-body terms (ΔE_3) in kcal mol^{-1} for DNA base trimers.

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
CCC (14)										
1	-48.27	-24.78	-25.00	1.23	0.28	-44.13	-22.72	-22.92	1.26	0.26
2	-47.86	-24.18	-24.49	0.89	-0.09	-43.83	-22.24	-22.46	0.88	-0.00
3	-46.27	-6.64	-10.83	-24.01	-4.79	-42.36	-5.68	-9.79	-22.06	-4.83
4	-46.06	-24.99	-22.49	1.07	0.36	-42.12	-22.88	-20.67	1.08	0.35
5	-42.78	-22.23	-7.78	-10.08	-2.70	-39.19	-20.43	-7.05	-9.00	-2.71
6	-35.47	-24.86	-10.96	0.44	-0.09	-32.32	-22.71	-10.01	0.46	-0.06
7	-43.98	-21.96	-9.52	-11.56	-0.94	-37.02	-19.86	-7.63	-8.57	-0.96
8	-42.78	-11.18	-7.00	-25.12	0.52	-35.97	-7.87	-5.64	-23.03	0.56
9	-42.28	-23.77	-15.07	-4.13	0.68	-35.86	-21.70	-11.51	-3.36	0.71
10	-41.25	-0.58	-24.71	-16.54	0.57	-35.60	-0.45	-22.71	-13.06	0.63
11	-43.02	-20.93	-7.90	-10.59	-3.60	-38.60	-18.88	-6.81	-9.27	-3.64
12	-29.34	-0.38	-16.09	-13.29	0.41	-22.78	-0.35	-12.81	-10.18	0.57
13	-43.48	-7.63	-12.88	-22.33	-0.63	-37.19	-6.75	-9.53	-20.15	-0.77
14	-36.28	-10.04	-11.14	-9.92	-5.17	-30.80	-8.27	-9.52	-7.95	-5.06
CGCplus (13)										
15	-80.49	2.59	-30.44	-48.70	-3.94	-75.97	2.58	-28.16	-46.45	-3.94
16	-77.16	0.90	-34.06	-48.70	4.70	-73.35	0.94	-32.68	-46.35	4.73
17	-81.04	-30.69	-44.17	0.56	-6.75	-76.45	-28.37	-42.13	0.83	-6.77
18	-75.60	0.26	-31.67	-48.63	4.44	-71.92	0.30	-30.41	-46.27	4.47
19	-74.82	1.42	-32.61	-48.74	5.12	-71.21	1.55	-31.35	-46.46	5.05
20	-74.01	2.64	-32.62	-48.83	4.80	-70.50	2.74	-31.46	-46.55	4.76
21	-76.28	1.22	-45.30	-37.27	5.07	-72.50	1.27	-43.50	-35.39	5.11
22	-71.67	0.51	-39.83	-37.10	4.74	-68.17	0.55	-38.30	-35.18	4.77
23	-71.33	-5.42	-23.63	-48.29	6.01	-63.52	-2.03	-21.52	-45.85	5.87
24	-64.49	-16.14	1.78	-50.36	0.23	-57.93	-12.41	1.82	-47.56	0.22

TABLE SII: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
25	-69.03	-4.08	-31.32	-38.89	5.26	-65.32	-3.14	-30.25	-37.16	5.23
26	-72.03	-6.53	-23.72	-47.88	6.09	-64.33	-3.43	-21.33	-45.49	5.92
27	-67.44	-18.51	-14.81	-37.96	3.84	-60.46	-16.39	-11.68	-36.13	3.73
GGG (12)										
28	-58.29	-16.35	-16.35	-16.35	-9.25	-54.50	-15.14	-15.14	-15.14	-9.08
29	-42.07	-20.52	-20.25	0.10	-1.41	-38.66	-18.78	-18.65	0.11	-1.35
30	-49.54	-1.05	-28.32	-19.98	-0.19	-44.68	-1.06	-25.68	-17.77	-0.16
31	-48.15	-14.32	-17.38	-10.71	-5.74	-43.32	-13.08	-15.07	-9.47	-5.71
32	-48.00	-18.51	-26.69	-1.81	-0.99	-43.19	-16.67	-24.25	-1.21	-1.07
33	-45.53	-11.12	-6.21	-26.83	-1.37	-41.15	-9.85	-5.12	-24.74	-1.44
34	-41.33	-12.24	-0.49	-28.14	-0.46	-37.44	-11.16	-0.49	-25.40	-0.39
35	-31.23	-0.76	-18.07	-11.95	-0.45	-20.91	-0.75	-13.07	-7.23	0.13
36	-51.35	-26.78	-13.23	-11.92	0.58	-41.63	-23.92	-9.07	-9.15	0.51
37	-51.01	-16.83	-13.51	-15.70	-4.97	-43.76	-15.00	-12.28	-11.61	-4.87
38	-50.66	-22.46	-14.89	-11.45	-1.86	-42.97	-19.58	-12.77	-8.72	-1.89
39	-55.39	-15.64	-15.64	-15.64	-8.47	-49.84	-13.84	-13.84	-13.84	-8.33
mAmUmU (12)										
40	-31.07	-15.78	0.63	-16.08	0.16	-27.44	-13.93	0.66	-14.30	0.13
42	-28.44	-4.70	-8.29	-15.63	0.18	-22.03	-3.31	-5.15	-13.86	0.28
43	-27.33	-13.91	-0.77	-12.55	-0.10	-18.96	-9.76	-0.78	-8.82	0.40
44	-24.65	-0.26	-10.48	-13.71	-0.20	-17.09	-0.23	-7.53	-9.52	0.19
45	-35.37	-13.18	-8.49	-13.58	-0.12	-27.79	-9.30	-6.65	-11.75	-0.09
46	-34.89	-12.43	-8.22	-14.22	-0.02	-27.40	-8.56	-6.46	-12.38	-0.00
47	-34.46	-13.91	-7.32	-13.17	-0.06	-26.89	-12.07	-5.61	-9.16	-0.06
48	-34.77	-13.03	-7.58	-14.23	0.07	-27.27	-9.06	-5.89	-12.39	0.08
49	-34.60	-13.28	-10.59	-10.65	-0.08	-26.67	-9.37	-8.80	-8.43	-0.07

TABLE SII: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
50	-30.00	-15.67	-3.79	-10.45	-0.10	-23.57	-13.82	-3.11	-6.56	-0.07
51	-29.15	-3.93	-10.25	-14.98	0.02	-23.41	-3.00	-7.27	-13.18	0.04
mCmCmC (12)										
52	-30.31	-5.74	0.36	-25.25	0.32	-27.13	-4.95	0.39	-22.92	0.35
53	-43.13	-13.12	-5.64	-24.94	0.57	-35.06	-9.11	-4.05	-22.53	0.63
54	-43.30	-24.95	-5.60	-13.14	0.39	-35.39	-22.62	-4.15	-9.11	0.49
55	-18.24	-0.64	-6.48	-11.13	0.01	-14.63	-0.52	-5.35	-8.82	0.06
56	-30.37	-0.71	-14.90	-14.92	0.17	-21.36	-0.66	-10.70	-10.65	0.65
57	-45.54	-23.70	-11.21	-10.26	-0.37	-37.51	-21.36	-7.09	-8.72	-0.34
58	-43.58	-14.42	-23.45	-6.40	0.68	-35.39	-10.16	-20.98	-4.94	0.68
59	-36.96	-11.01	-12.75	-11.67	-1.52	-30.47	-7.41	-11.33	-10.20	-1.53
60	-35.44	-10.60	-12.02	-11.28	-1.54	-27.21	-9.06	-9.07	-7.75	-1.33
61	-36.50	-13.17	-14.75	-8.10	-0.48	-28.28	-10.71	-11.15	-6.12	-0.31
62	-29.40	-10.79	-10.40	-9.31	1.10	-23.43	-7.37	-8.75	-8.38	1.07
63	-39.55	-12.99	-10.62	-11.32	-4.61	-32.46	-10.61	-8.50	-8.91	-4.44
mTmUmU (12)										
64	-21.67	-0.06	-9.21	-12.22	-0.18	-18.92	-0.05	-7.96	-10.73	-0.18
65	-21.12	-12.20	-8.59	-0.14	-0.19	-18.41	-10.72	-7.37	-0.12	-0.20
66	-25.55	-9.39	-11.89	-4.03	-0.25	-19.02	-5.87	-10.37	-2.66	-0.12
67	-23.37	-12.22	-6.28	-4.63	-0.24	-19.63	-10.70	-4.85	-3.86	-0.21
68	-22.48	-0.04	-10.40	-12.03	0.00	-15.66	-0.03	-7.38	-8.53	0.28
69	-21.16	-11.51	0.18	-9.78	-0.06	-14.11	-8.17	0.19	-6.35	0.22
70	-32.04	-9.98	-9.79	-12.36	0.09	-24.86	-6.90	-7.46	-10.61	0.11
71	-31.99	-12.28	-9.86	-9.94	0.09	-24.87	-10.56	-6.89	-7.52	0.11
72	-28.65	-4.87	-11.99	-11.48	-0.31	-22.09	-3.57	-10.19	-8.04	-0.29
73	-26.94	-9.63	-11.88	-5.20	-0.23	-20.23	-6.29	-10.24	-3.52	-0.18
74	-23.81	-12.04	-8.19	-3.51	-0.07	-18.22	-10.43	-5.00	-2.79	-0.00

TABLE SII: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
75	-31.05	-10.07	-8.92	-12.18	0.12	-23.86	-6.89	-6.62	-10.48	0.13
mUmUmU (12)										
76	-22.00	-12.01	-4.28	-5.56	-0.16	-19.12	-10.60	-3.71	-4.65	-0.16
77	-21.47	-12.02	-9.16	-0.07	-0.23	-18.75	-10.57	-7.95	-0.07	-0.17
78	-16.22	-9.19	0.11	-7.11	-0.02	-13.93	-7.95	0.11	-6.05	-0.03
79	-28.25	-7.59	-12.11	-8.76	0.21	-21.91	-5.45	-10.56	-6.16	0.26
80	-27.72	-6.03	-12.01	-9.77	0.08	-21.35	-4.19	-10.55	-6.75	0.14
81	-26.21	-9.62	-11.80	-4.64	-0.15	-20.91	-6.44	-10.25	-4.08	-0.14
82	-25.25	-9.62	-4.05	-11.48	-0.10	-19.98	-6.44	-3.51	-9.94	-0.09
83	-17.39	0.50	-8.86	-8.86	-0.17	-11.20	0.51	-5.90	-5.92	0.10
84	-30.74	-9.87	-8.96	-12.02	0.11	-23.70	-6.83	-6.64	-10.36	0.12
85	-25.52	-12.77	-3.84	-8.83	-0.09	-19.94	-11.11	-3.05	-5.75	-0.03
86	-31.82	-9.84	-12.20	-9.88	0.09	-24.77	-7.49	-10.49	-6.92	0.11
87	-27.61	-12.07	-11.05	-4.13	-0.36	-21.95	-10.23	-8.10	-3.27	-0.34
TAT (12)										
88	-37.31	-19.27	-0.65	-17.41	0.02	-33.82	-17.58	-0.63	-15.65	0.04
89	-34.47	-12.01	-2.80	-19.52	-0.13	-31.01	-10.44	-2.43	-17.97	-0.17
90	-36.60	-0.51	-15.57	-20.01	-0.51	-33.26	-0.52	-14.00	-18.25	-0.49
91	-30.72	0.70	-16.12	-15.49	0.19	-27.20	0.73	-14.38	-13.70	0.16
92	-32.60	-8.86	-7.60	-16.46	0.32	-26.87	-7.56	-4.83	-14.83	0.35
93	-24.26	-0.52	-11.92	-11.56	-0.26	-16.38	-0.52	-8.10	-7.97	0.21
94	-22.46	-11.06	-10.81	-0.39	-0.20	-15.33	-7.81	-7.31	-0.35	0.14
95	-35.55	-14.98	-10.78	-10.18	0.39	-28.56	-13.31	-7.36	-8.27	0.38
96	-35.28	-14.79	-10.01	-10.88	0.40	-28.30	-13.16	-8.12	-7.42	0.40
97	-34.11	-8.56	-9.83	-15.92	0.20	-27.82	-7.21	-6.56	-14.27	0.22
98	-32.64	-6.34	-10.16	-16.39	0.25	-25.87	-4.43	-6.99	-14.72	0.26
99	-33.34	-16.65	-10.30	-6.46	0.08	-27.07	-14.85	-8.00	-4.27	0.05

TABLE SII: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
UUA (16)										
100	-37.16	-19.08	-0.66	-17.43	0.02	-33.71	-17.43	-0.65	-15.67	0.04
101	-35.98	-15.74	-19.42	-0.77	-0.05	-32.70	-14.12	-17.77	-0.78	-0.03
102	-36.33	0.06	-19.75	-16.16	-0.49	-32.84	0.06	-18.05	-14.37	-0.48
103	-36.43	-0.46	-15.59	-19.92	-0.46	-33.15	-0.48	-14.04	-18.18	-0.45
104	-35.56	-19.21	-0.61	-15.79	0.05	-32.03	-17.55	-0.58	-13.97	0.07
105	-34.83	-15.40	-17.00	-2.67	0.24	-31.18	-13.70	-15.37	-2.32	0.21
106	-30.78	-15.61	-16.13	0.75	0.21	-27.20	-13.79	-14.37	0.79	0.17
107	-30.76	-15.58	-16.02	0.66	0.19	-27.15	-13.77	-14.22	0.69	0.15
108	-28.82	-16.49	-9.26	-2.75	-0.32	-25.44	-14.72	-8.00	-2.35	-0.38
109	-27.43	-16.01	-2.25	-8.57	-0.60	-24.11	-14.22	-1.92	-7.30	-0.67
110	-29.85	-4.86	-17.34	-8.09	0.43	-24.62	-2.28	-15.73	-7.00	0.40
111	-21.56	-0.32	-10.86	-10.16	-0.22	-14.62	-0.32	-7.46	-7.05	0.21
112	-19.82	-9.20	-0.08	-10.29	-0.25	-13.35	-6.44	-0.05	-6.91	0.04
113	-35.01	-15.25	-9.66	-10.49	0.39	-28.39	-13.60	-7.89	-7.30	0.40
114	-34.47	-14.59	-10.61	-9.70	0.42	-27.80	-13.00	-7.32	-7.90	0.43
115	-31.97	-3.42	-10.17	-18.50	0.12	-25.95	-2.21	-7.15	-16.83	0.24
UUT (12)										
116	-35.68	-15.73	-0.85	-19.03	-0.07	-32.40	-14.12	-0.86	-17.38	-0.05
117	-35.56	-0.89	-15.62	-19.03	-0.03	-32.30	-0.89	-14.03	-17.37	-0.01
118	-35.01	-3.10	-12.32	-19.56	-0.03	-31.53	-2.68	-10.79	-17.97	-0.10
119	-34.93	-19.47	-3.18	-12.24	-0.04	-31.49	-17.89	-2.76	-10.75	-0.10
120	-31.27	-12.45	0.34	-19.14	-0.02	-28.39	-11.20	0.34	-17.50	-0.04
121	-17.23	0.58	-8.83	-8.74	-0.24	-11.40	0.58	-6.03	-5.96	0.00
122	-16.83	-8.40	-8.77	0.61	-0.27	-11.12	-5.88	-5.88	0.62	0.03
123	-31.54	-9.68	-14.45	-7.79	0.38	-25.35	-7.97	-12.56	-5.27	0.45
124	-30.27	-6.66	-14.03	-9.93	0.36	-24.34	-4.38	-12.30	-8.14	0.49

TABLE SII: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
125	-20.97	-6.59	-4.10	-9.94	-0.35	-15.24	-4.06	-2.16	-8.71	-0.31
126	-32.61	-10.70	-10.81	-10.74	-0.37	-27.36	-8.98	-9.04	-8.98	-0.35
127	-29.03	-6.66	-13.64	-9.01	0.27	-24.15	-5.72	-11.83	-6.89	0.29
UUU (14)										
128	-35.58	-18.95	-0.88	-15.71	-0.04	-32.31	-17.30	-0.89	-14.10	-0.02
129	-34.76	-12.10	-19.45	-3.13	-0.09	-31.33	-10.60	-17.89	-2.70	-0.14
130	-31.11	0.35	-19.04	-12.44	0.02	-28.24	0.35	-17.41	-11.18	-0.00
131	-27.63	-15.02	0.03	-12.51	-0.14	-24.86	-13.51	0.04	-11.24	-0.15
132	-28.90	-15.83	-0.40	-12.42	-0.24	-26.02	-14.23	-0.39	-11.18	-0.22
133	-29.63	-5.90	-18.73	-5.26	0.26	-24.11	-4.69	-17.11	-2.55	0.23
134	-23.11	-12.92	-7.99	-1.76	-0.44	-19.42	-11.39	-6.65	-0.94	-0.45
135	-22.14	-12.20	-8.25	-1.34	-0.35	-18.78	-10.60	-7.26	-0.69	-0.23
136	-16.77	-7.40	-9.04	-0.23	-0.10	-11.21	-4.66	-6.45	-0.23	0.13
137	-30.33	-14.65	-6.65	-9.55	0.52	-24.32	-12.82	-4.22	-7.77	0.48
138	-29.10	-4.12	-18.25	-6.85	0.12	-23.71	-3.29	-16.46	-4.07	0.11
139	-27.61	-16.83	-8.19	-3.02	0.43	-21.81	-14.88	-5.34	-1.95	0.35
140	-29.23	-4.89	-7.37	-17.16	0.20	-24.13	-2.31	-6.43	-15.69	0.31
141	-32.70	-10.77	-10.77	-10.77	-0.39	-27.50	-9.04	-9.04	-9.04	-0.38

TABLE SIII: HF/TZV(2df,2pd) interaction energies (ΔE), two- (ΔE_{12}, ΔE_{23}, ΔE_{13}), and three-body terms (ΔE_3) in kcal mol^{-1} for DNA base trimers.

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
CCC (14)										
1	-42.26	-21.45	-23.21	1.95	0.44	-41.55	-21.07	-22.88	1.96	0.44
2	-40.38	-20.58	-21.05	1.34	-0.09	-39.84	-20.43	-20.76	1.24	0.12
3	-38.36	-4.51	-8.45	-20.86	-4.54	-37.60	-4.27	-8.25	-20.48	-4.59
4	-38.80	-23.18	-17.54	1.41	0.52	-38.09	-22.82	-17.18	1.41	0.50
5	-33.64	-17.25	-6.64	-7.39	-2.35	-32.94	-16.91	-6.47	-7.18	-2.38
6	-31.40	-22.99	-9.09	0.61	0.07	-30.82	-22.63	-8.89	0.61	0.09
7	-24.15	-18.25	-2.54	-2.54	-0.81	-22.66	-17.73	-2.09	-1.83	-1.01
8	-23.76	0.66	-2.21	-23.22	1.01	-22.33	1.46	-1.84	-22.79	0.85
9	-22.62	-20.24	-1.21	-2.34	1.16	-21.22	-19.77	-0.38	-2.08	1.00
10	-24.91	-0.20	-21.21	-4.37	0.87	-23.78	-0.22	-20.90	-3.54	0.88
11	-35.13	-17.06	-5.88	-8.73	-3.46	-34.15	-16.61	-5.60	-8.39	-3.55
12	-7.22	-0.19	-4.63	-3.18	0.78	-5.75	-0.16	-3.84	-2.44	0.69
13	-26.39	-6.18	0.30	-20.24	-0.28	-25.06	-5.90	1.05	-19.74	-0.46
14	-21.45	-5.18	-6.96	-4.26	-5.04	-20.13	-4.72	-6.60	-3.78	-5.03
CGCplus (13)										
15	-70.58	2.88	-26.51	-43.60	-3.34	-69.84	2.86	-26.13	-43.23	-3.34
16	-69.56	1.24	-31.85	-43.75	4.80	-68.95	1.26	-31.61	-43.40	4.80
17	-70.54	-26.75	-39.04	1.39	-6.15	-69.77	-26.35	-38.69	1.44	-6.17
18	-68.90	0.41	-30.12	-43.65	4.46	-68.32	0.42	-29.91	-43.30	4.46
19	-66.01	1.97	-29.09	-44.07	5.18	-65.46	2.02	-28.88	-43.71	5.12
20	-65.96	3.71	-30.29	-44.14	4.76	-65.40	3.75	-30.09	-43.80	4.74
21	-68.43	1.62	-40.83	-34.43	5.21	-67.82	1.64	-40.54	-34.13	5.21
22	-64.48	0.73	-35.81	-34.18	4.77	-63.91	0.75	-35.56	-33.88	4.77
23	-45.22	9.69	-17.96	-43.24	6.30	-43.75	10.48	-17.48	-42.76	6.00
24	-44.03	-2.82	3.25	-45.03	0.57	-42.79	-1.99	3.23	-44.47	0.44

TABLE SIII: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
25	-59.26	-0.63	-29.17	-34.84	5.38	-58.62	-0.37	-29.00	-34.63	5.38
26	-46.30	6.06	-15.97	-42.82	6.43	-44.86	6.81	-15.47	-42.32	6.12
27	-44.64	-13.73	-0.55	-34.28	3.92	-43.40	-13.25	0.05	-33.90	3.71
GGG (12)										
28	-54.40	-15.20	-15.20	-15.20	-8.80	-53.65	-14.97	-14.97	-14.97	-8.73
29	-35.08	-17.19	-17.09	0.31	-1.10	-34.39	-16.82	-16.78	0.31	-1.09
30	-39.70	-1.35	-24.69	-13.39	-0.27	-38.78	-1.36	-24.19	-12.98	-0.26
31	-37.64	-12.30	-11.46	-8.29	-5.60	-36.66	-12.02	-10.95	-8.04	-5.65
32	-38.52	-14.82	-23.43	0.63	-0.90	-37.49	-14.40	-22.92	0.81	-0.98
33	-36.04	-7.67	-2.16	-24.92	-1.29	-35.15	-7.37	-1.92	-24.52	-1.34
34	-33.89	-8.68	-0.59	-24.17	-0.45	-33.09	-8.45	-0.58	-23.63	-0.42
35	12.86	-0.21	3.33	9.59	0.14	14.69	-0.20	4.31	10.51	0.07
36	-16.00	-21.95	5.94	-0.72	0.73	-14.14	-21.32	6.84	-0.11	0.46
37	-29.01	-12.61	-12.31	0.60	-4.69	-27.55	-12.19	-12.04	1.43	-4.75
38	-27.14	-16.55	-8.62	-0.33	-1.65	-25.38	-15.78	-8.09	0.27	-1.79
39	-44.91	-12.25	-12.25	-12.25	-8.16	-43.59	-11.82	-11.82	-11.82	-8.13
mAmUmU (12)										
40	-20.97	-10.94	0.99	-11.17	0.15	-20.28	-10.58	0.99	-10.83	0.15
42	-3.89	0.80	5.65	-10.52	0.19	-2.65	1.16	6.27	-10.16	0.08
43	10.82	5.68	-0.57	5.26	0.44	12.24	6.43	-0.56	5.97	0.40
44	9.12	0.20	2.41	6.19	0.31	10.44	0.23	3.03	6.95	0.23
45	-7.49	4.43	-3.67	-8.00	-0.25	-6.10	5.19	-3.32	-7.61	-0.36
46	-7.00	5.68	-3.90	-8.63	-0.14	-5.65	6.41	-3.56	-8.24	-0.26
47	-6.33	-8.32	-2.82	5.01	-0.20	-4.95	-7.92	-2.48	5.80	-0.34
48	-6.67	5.46	-3.50	-8.60	-0.03	-5.32	6.22	-3.17	-8.20	-0.17
49	-4.95	4.43	-5.79	-3.57	-0.02	-3.51	5.21	-5.49	-3.06	-0.16

TABLE SIII: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
50	-4.73	-10.39	-1.74	7.64	-0.24	-3.51	-10.02	-1.57	8.40	-0.32
51	-8.75	-0.85	2.00	-9.90	-0.01	-7.56	-0.54	2.61	-9.51	-0.12
mCmCmC (12)										
52	-20.33	-3.59	0.66	-17.78	0.38	-19.64	-3.37	0.67	-17.32	0.38
53	-11.81	3.20	1.53	-17.17	0.63	-10.19	4.09	1.89	-16.62	0.46
54	-13.08	-17.50	0.49	3.39	0.53	-11.48	-16.96	0.84	4.28	0.36
55	-6.90	0.01	-3.00	-3.97	0.05	-6.07	0.04	-2.71	-3.42	0.02
56	6.63	-0.30	2.97	3.11	0.85	8.39	-0.26	3.86	4.01	0.77
57	-15.13	-16.39	6.10	-4.80	-0.04	-13.50	-15.86	7.01	-4.41	-0.24
58	-13.19	2.88	-15.61	-1.19	0.74	-11.57	3.79	-15.05	-0.83	0.53
59	-14.64	3.43	-9.35	-7.39	-1.33	-13.24	4.26	-8.99	-7.06	-1.45
60	-3.74	-5.80	-1.79	5.32	-1.47	-2.06	-5.40	-1.12	6.06	-1.60
61	-6.98	-4.33	-1.81	-0.55	-0.30	-5.30	-3.69	-1.07	-0.10	-0.44
62	-8.29	3.04	-5.10	-7.43	1.20	-6.94	3.79	-4.67	-7.18	1.11
63	-14.59	-4.62	-3.37	-2.21	-4.39	-13.01	-4.07	-2.86	-1.66	-4.43
mTmUmU (12)										
64	-15.67	0.05	-6.78	-8.75	-0.18	-15.16	0.05	-6.53	-8.51	-0.18
65	-14.93	-8.75	-5.93	-0.05	-0.19	-14.42	-8.49	-5.68	-0.04	-0.21
66	-0.67	5.79	-7.97	1.71	-0.19	0.47	6.45	-7.71	2.00	-0.27
67	-13.12	-8.64	-1.03	-3.24	-0.22	-12.39	-8.38	-0.69	-3.07	-0.25
68	5.68	0.44	2.58	2.23	0.43	6.90	0.45	3.21	2.88	0.35
69	9.03	3.02	0.66	5.00	0.34	10.27	3.66	0.68	5.65	0.29
70	-8.25	2.97	-3.15	-8.25	0.19	-6.99	3.57	-2.69	-7.96	0.09
71	-8.45	-8.11	2.26	-2.77	0.18	-7.18	-7.83	2.86	-2.29	0.08
72	-5.78	-0.34	-7.69	2.55	-0.31	-4.63	-0.07	-7.37	3.21	-0.40
73	-2.04	4.47	-7.88	1.62	-0.25	-0.88	5.10	-7.59	1.95	-0.33
74	-3.79	-8.30	5.96	-1.51	0.06	-2.77	-8.01	6.57	-1.32	-0.01

TABLE SIII: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
75	-6.64	3.40	-2.23	-8.01	0.20	-5.40	4.01	-1.77	-7.72	0.08
mUmUmU (12)										
76	-16.32	-8.82	-4.07	-3.30	-0.13	-15.72	-8.56	-3.93	-3.07	-0.16
77	-15.52	-8.60	-6.69	0.04	-0.26	-15.04	-8.38	-6.52	0.03	-0.17
78	-11.25	-6.81	0.17	-4.58	-0.03	-10.78	-6.55	0.17	-4.36	-0.03
79	-7.74	-0.25	-8.42	0.58	0.35	-6.56	0.18	-8.15	1.13	0.27
80	-8.10	-0.76	-8.47	0.97	0.16	-6.90	-0.34	-8.21	1.57	0.09
81	-8.80	3.51	-8.40	-3.90	-0.01	-7.80	4.12	-8.10	-3.72	-0.10
82	-7.25	3.52	-2.91	-7.88	0.02	-6.26	4.13	-2.74	-7.59	-0.06
83	8.40	1.13	3.62	3.50	0.15	9.50	1.14	4.18	4.06	0.11
84	-7.22	2.71	-2.17	-7.96	0.20	-5.97	3.32	-1.71	-7.67	0.08
85	-6.78	-9.47	-1.89	4.59	-0.01	-5.75	-9.17	-1.68	5.19	-0.09
86	-8.94	-3.12	-8.18	2.17	0.19	-7.67	-2.65	-7.89	2.78	0.09
87	-9.26	-7.80	0.71	-1.84	-0.33	-8.21	-7.48	1.33	-1.66	-0.39
TAT (12)										
88	-30.04	-16.74	-0.50	-12.84	0.03	-29.46	-16.48	-0.49	-12.52	0.03
89	-25.77	-8.60	-1.81	-15.27	-0.08	-25.16	-8.34	-1.71	-14.99	-0.12
90	-27.20	-0.65	-10.77	-15.24	-0.54	-26.61	-0.66	-10.47	-14.94	-0.53
91	-20.86	1.11	-11.38	-10.77	0.19	-20.20	1.13	-11.05	-10.44	0.16
92	-13.07	-5.75	4.52	-12.13	0.29	-12.07	-5.49	5.06	-11.83	0.20
93	10.11	-0.21	5.27	4.89	0.16	11.47	-0.20	5.99	5.57	0.11
94	8.34	2.40	5.60	0.15	0.20	9.58	3.04	6.24	0.18	0.12
95	-12.19	-11.69	3.21	-4.04	0.35	-10.94	-11.42	3.90	-3.66	0.23
96	-11.82	-11.36	-4.24	3.40	0.38	-10.58	-11.08	-3.86	4.11	0.26
97	-12.44	-5.60	4.25	-11.33	0.24	-11.34	-5.34	4.87	-11.02	0.15
98	-7.67	-0.43	4.10	-11.54	0.21	-6.45	-0.03	4.69	-11.21	0.10
99	-12.96	-13.31	-1.89	2.04	0.20	-11.79	-12.97	-1.42	2.53	0.07

TABLE SIII: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
UUA (16)										
100	-30.39	-16.88	-0.52	-13.03	0.03	-29.81	-16.63	-0.51	-12.70	0.03
101	-29.09	-13.21	-14.93	-0.85	-0.09	-28.54	-12.94	-14.65	-0.85	-0.09
102	-27.10	0.11	-15.22	-11.39	-0.60	-26.46	0.11	-14.93	-11.04	-0.60
103	-27.37	-0.60	-10.97	-15.30	-0.50	-26.79	-0.61	-10.67	-15.01	-0.50
104	-28.27	-17.01	-0.35	-11.04	0.12	-27.67	-16.75	-0.34	-10.69	0.12
105	-26.68	-12.62	-12.69	-1.73	0.35	-26.02	-12.34	-12.36	-1.63	0.31
106	-21.01	-10.92	-11.47	1.18	0.20	-20.30	-10.58	-11.12	1.22	0.17
107	-20.87	-10.92	-11.16	1.03	0.18	-20.17	-10.58	-10.81	1.05	0.16
108	-20.50	-11.75	-7.02	-1.53	-0.20	-19.79	-11.39	-6.73	-1.41	-0.26
109	-19.28	-11.35	-1.17	-6.24	-0.53	-18.62	-11.00	-1.07	-5.96	-0.58
110	-12.57	5.30	-13.10	-5.06	0.29	-11.56	5.83	-12.78	-4.79	0.19
111	8.03	-0.09	4.15	3.84	0.14	9.30	-0.08	4.82	4.46	0.10
112	6.72	1.46	0.34	4.83	0.09	7.93	2.02	0.37	5.51	0.04
113	-13.74	-12.41	-4.07	2.35	0.38	-12.53	-12.13	-3.71	3.03	0.28
114	-12.50	-11.37	2.81	-4.34	0.40	-11.29	-11.10	3.50	-3.97	0.28
115	-8.99	1.31	3.27	-13.40	-0.18	-8.11	1.40	3.89	-13.30	-0.09
UUT (12)										
116	-31.04	-13.20	-1.06	-16.68	-0.10	-30.53	-12.94	-1.06	-16.43	-0.10
117	-30.78	-1.12	-12.93	-16.66	-0.07	-30.28	-1.12	-12.68	-16.41	-0.07
118	-29.39	-2.95	-9.02	-17.51	0.09	-28.78	-2.85	-8.73	-17.24	0.05
119	-29.35	-17.55	-2.92	-8.96	0.07	-28.78	-17.30	-2.82	-8.70	0.04
120	-27.38	-10.93	0.47	-16.88	-0.04	-26.90	-10.70	0.48	-16.63	-0.05
121	6.94	1.23	2.92	2.82	-0.02	8.00	1.23	3.47	3.36	-0.06
122	7.29	2.13	3.75	1.38	0.03	8.35	2.68	4.31	1.39	-0.03
123	-12.61	-5.58	-10.60	3.14	0.43	-11.69	-5.41	-10.28	3.53	0.47
124	-11.82	3.69	-9.98	-5.88	0.36	-11.07	3.93	-9.85	-5.67	0.53

TABLE SIII: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
125	-1.09	3.34	3.52	-7.54	-0.41	-0.02	3.87	3.92	-7.28	-0.53
126	-19.39	-6.44	-6.27	-6.17	-0.52	-18.42	-6.11	-5.93	-5.84	-0.53
127	-17.96	-4.48	-10.02	-3.68	0.22	-17.11	-4.28	-9.72	-3.28	0.15
UUU (14)										
128	-31.10	-16.72	-1.11	-13.19	-0.07	-30.59	-16.48	-1.11	-12.94	-0.07
129	-29.32	-8.80	-17.56	-2.98	0.02	-28.74	-8.54	-17.31	-2.88	-0.01
130	-27.35	0.48	-16.92	-10.92	-0.00	-26.88	0.49	-16.67	-10.68	-0.01
131	-23.33	-12.24	0.05	-10.98	-0.15	-22.86	-12.01	0.05	-10.74	-0.16
132	-24.99	-13.38	-0.50	-10.84	-0.27	-24.49	-13.12	-0.50	-10.62	-0.26
133	-13.80	-2.87	-16.57	5.36	0.29	-12.78	-2.60	-16.28	5.92	0.19
134	-15.03	-10.05	-5.09	0.47	-0.37	-14.32	-9.77	-4.80	0.67	-0.42
135	-14.66	-9.21	-6.00	0.91	-0.35	-14.18	-8.99	-5.95	0.95	-0.20
136	4.62	3.04	1.45	0.02	0.11	5.69	3.59	2.01	0.03	0.06
137	-12.68	-11.15	3.40	-5.54	0.61	-11.63	-10.84	3.93	-5.21	0.50
138	-13.38	-1.85	-15.50	4.11	-0.14	-12.50	-1.72	-15.19	4.56	-0.15
139	-9.32	-13.38	2.81	0.93	0.31	-8.27	-13.03	3.38	1.19	0.18
140	-14.07	5.56	-5.05	-14.69	0.11	-13.33	6.10	-5.04	-14.63	0.24
141	-19.98	-6.48	-6.48	-6.48	-0.53	-19.01	-6.15	-6.15	-6.15	-0.56

TABLE SIV: B97-D/TZV(2df,2pd) interaction energies (ΔE), two- (ΔE_{12}, ΔE_{23}, ΔE_{13}), and three-body terms (ΔE_3) in kcal mol^{-1} for DNA base trimers.

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
CCC (14)										
1	-49.98	-25.79	-25.70	1.09	0.41	-48.67	-25.08	-25.05	1.10	0.36
2	-50.03	-25.31	-25.57	0.77	0.08	-48.68	-24.65	-24.87	0.79	0.06
3	-46.61	-6.37	-10.86	-24.92	-4.46	-45.25	-5.93	-10.51	-24.25	-4.56
4	-47.89	-25.68	-23.64	0.99	0.44	-46.64	-25.03	-23.02	1.00	0.41
5	-43.59	-23.39	-7.45	-10.19	-2.56	-42.35	-22.81	-7.11	-9.82	-2.61
6	-36.01	-25.60	-10.86	0.45	0.00	-34.91	-24.95	-10.46	0.48	0.02
7	-44.50	-23.02	-9.75	-11.06	-0.67	-42.52	-22.23	-9.18	-10.20	-0.91
8	-42.76	-10.96	-6.98	-25.93	1.12	-40.90	-10.08	-6.48	-25.26	0.93
9	-43.38	-24.78	-15.48	-4.36	1.24	-41.48	-24.04	-14.51	-3.99	1.06
10	-42.31	-0.89	-25.76	-16.67	1.01	-40.61	-0.76	-25.08	-15.68	0.91
11	-44.30	-21.95	-8.61	-10.30	-3.43	-42.75	-21.23	-8.14	-9.82	-3.56
12	-28.96	-0.58	-16.31	-12.77	0.70	-27.19	-0.54	-15.36	-11.95	0.67
13	-43.52	-7.47	-13.07	-22.79	-0.19	-41.67	-7.01	-12.18	-22.04	-0.44
14	-35.84	-9.90	-10.95	-9.74	-5.26	-34.01	-9.30	-10.40	-9.09	-5.22
CGCplus (13)										
15	-83.65	2.32	-31.58	-50.48	-3.92	-82.33	2.29	-30.88	-49.80	-3.93
16	-79.52	0.85	-35.86	-49.67	5.17	-78.45	0.88	-35.42	-49.09	5.18
17	-83.58	-31.80	-45.57	0.24	-6.46	-82.20	-31.08	-44.92	0.34	-6.54
18	-77.53	0.23	-33.02	-49.59	4.85	-76.54	0.26	-32.64	-49.01	4.86
19	-75.98	1.34	-33.58	-49.62	5.88	-74.97	1.48	-33.20	-49.04	5.79
20	-74.67	2.74	-33.12	-49.70	5.40	-73.69	2.83	-32.75	-49.12	5.36
21	-79.12	1.13	-46.85	-39.05	5.65	-78.06	1.18	-46.34	-38.56	5.66
22	-74.12	0.48	-40.98	-38.84	5.22	-73.12	0.52	-40.52	-38.34	5.23
23	-70.07	-3.72	-23.86	-49.22	6.73	-68.11	-2.75	-23.21	-48.50	6.35
24	-65.17	-15.55	1.14	-51.38	0.62	-63.55	-14.61	1.19	-50.55	0.43

TABLE SIV: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
25	-70.27	-4.36	-31.96	-39.92	5.97	-69.07	-3.89	-31.55	-39.43	5.80
26	-71.33	-5.35	-23.82	-48.88	6.72	-69.45	-4.45	-23.18	-48.18	6.36
27	-67.45	-19.55	-15.15	-37.40	4.65	-65.75	-18.79	-14.44	-36.85	4.33
GGG (12)										
28	-57.93	-15.96	-15.97	-15.97	-10.03	-56.47	-15.52	-15.52	-15.52	-9.92
29	-43.33	-21.12	-20.80	0.01	-1.42	-42.02	-20.43	-20.21	0.01	-1.40
30	-51.82	-1.18	-29.64	-20.83	-0.17	-50.25	-1.19	-28.81	-20.09	-0.16
31	-49.49	-14.24	-17.87	-11.08	-6.30	-47.90	-13.70	-17.16	-10.67	-6.36
32	-49.79	-18.90	-27.86	-2.19	-0.84	-48.06	-18.16	-27.06	-1.88	-0.97
33	-47.03	-10.94	-6.94	-27.95	-1.19	-45.44	-10.41	-6.51	-27.23	-1.29
34	-42.45	-12.20	-0.50	-29.36	-0.39	-41.11	-11.76	-0.50	-28.50	-0.34
[a]	-42.45	-12.20	-0.50	-29.36	-0.39	-41.10	-11.76	-0.50	-28.50	-0.34
[b]	-42.45	-12.20	-0.50	-29.36	-0.39	-41.10	-11.76	-0.50	-28.50	-0.34
[c]	-42.45	-12.20	-0.50	-29.36	-0.39	-41.10	-11.76	-0.50	-28.50	-0.34
35	-29.18	-0.99	-17.19	-11.19	0.18	-27.03	-0.97	-16.03	-10.17	0.14
36	-50.16	-27.92	-11.80	-11.49	1.06	-47.71	-26.97	-10.76	-10.67	0.69
37	-50.40	-17.29	-13.16	-14.60	-5.35	-48.32	-16.62	-12.70	-13.59	-5.42
38	-52.46	-23.57	-15.50	-11.56	-1.84	-49.99	-22.51	-14.75	-10.74	-1.99
39	-57.35	-16.00	-16.00	-16.00	-9.35	-55.24	-15.32	-15.32	-15.32	-9.27
mAmUmU (12)										
40	-33.05	-17.16	0.63	-16.79	0.27	-31.77	-16.53	0.66	-16.13	0.23
42	-28.97	-5.32	-7.81	-16.50	0.66	-27.29	-4.88	-7.06	-15.83	0.48
43	-26.01	-13.54	-1.03	-11.85	0.41	-24.36	-12.68	-1.03	-11.08	0.42
44	-24.10	-0.52	-10.62	-13.25	0.29	-22.57	-0.49	-9.93	-12.39	0.24
45	-34.71	-12.39	-8.03	-14.37	0.08	-32.80	-11.52	-7.49	-13.70	-0.09
46	-34.28	-11.72	-7.76	-15.03	0.23	-32.40	-10.89	-7.21	-14.35	0.06
47	-33.84	-14.45	-7.12	-12.42	0.15	-31.91	-13.74	-6.59	-11.52	-0.06

TABLE SIV: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
48	-34.13	-12.36	-7.41	-14.77	0.41	-32.25	-11.50	-6.88	-14.07	0.21
49	-33.62	-12.64	-10.94	-10.23	0.19	-31.68	-11.73	-10.42	-9.52	-0.02
50	-30.82	-16.70	-4.34	-9.93	0.16	-29.15	-16.02	-4.07	-9.06	-0.01
51	-30.23	-4.44	-10.48	-15.70	0.40	-28.59	-4.04	-9.75	-15.01	0.21
mCmCmC (12)										
52	-32.00	-5.89	0.18	-26.68	0.38	-30.83	-5.50	0.20	-25.90	0.38
53	-44.00	-12.34	-6.29	-26.31	0.94	-41.93	-11.34	-5.85	-25.44	0.70
54	-44.38	-26.28	-6.23	-12.75	0.88	-42.32	-25.42	-5.79	-11.75	0.63
55	-19.70	-1.06	-6.94	-11.85	0.15	-18.61	-1.02	-6.51	-11.20	0.11
56	-29.01	-1.12	-14.39	-14.29	0.78	-27.02	-1.07	-13.40	-13.30	0.76
57	-47.41	-25.09	-12.02	-10.43	0.14	-45.39	-24.26	-11.12	-9.84	-0.16
58	-45.17	-14.26	-24.85	-7.09	1.04	-43.13	-13.24	-23.98	-6.65	0.74
59	-37.28	-11.35	-12.95	-11.70	-1.27	-35.56	-10.53	-12.43	-11.15	-1.46
60	-35.70	-10.80	-12.08	-11.73	-1.09	-33.68	-10.24	-11.24	-10.97	-1.23
61	-35.89	-13.49	-14.16	-8.38	0.15	-33.75	-12.65	-13.32	-7.74	-0.04
62	-29.80	-11.04	-11.14	-9.02	1.40	-28.13	-10.21	-10.57	-8.61	1.26
63	-39.86	-13.04	-10.89	-11.57	-4.36	-37.95	-12.40	-10.28	-10.92	-4.36
mTmUmU (12)										
64	-21.74	-0.07	-9.45	-12.01	-0.20	-20.78	-0.07	-8.96	-11.55	-0.21
65	-20.90	-12.00	-8.51	-0.16	-0.23	-19.97	-11.54	-8.05	-0.15	-0.24
66	-25.21	-8.96	-11.85	-4.51	0.11	-23.66	-8.14	-11.37	-4.12	-0.03
67	-24.19	-12.08	-6.94	-5.05	-0.12	-23.07	-11.59	-6.53	-4.75	-0.19
68	-22.63	-0.18	-10.44	-12.39	0.38	-21.15	-0.16	-9.73	-11.58	0.33
69	-20.74	-11.85	0.02	-9.23	0.32	-19.21	-11.11	0.04	-8.42	0.28
70	-31.77	-9.95	-9.31	-12.85	0.34	-30.01	-9.23	-8.65	-12.32	0.19
71	-31.74	-12.76	-9.84	-9.47	0.34	-29.96	-12.24	-9.11	-8.79	0.18
72	-29.86	-5.66	-12.45	-11.68	-0.07	-28.30	-5.30	-11.89	-10.90	-0.22

TABLE SIV: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
73	-27.02	-9.19	-11.81	-6.05	0.03	-25.45	-8.43	-11.30	-5.61	-0.11
74	-23.26	-11.89	-7.88	-3.73	0.24	-21.82	-11.39	-7.12	-3.43	0.12
75	-30.38	-9.97	-8.53	-12.22	0.34	-28.66	-9.24	-7.88	-11.71	0.17
mUmUmU (12)										
76	-22.35	-11.75	-4.36	-6.18	-0.06	-21.29	-11.28	-4.09	-5.82	-0.10
77	-21.53	-11.82	-9.44	-0.09	-0.19	-20.58	-11.35	-8.95	-0.08	-0.19
78	-16.13	-9.40	0.11	-6.82	-0.02	-15.21	-8.91	0.11	-6.39	-0.03
79	-28.27	-7.76	-12.40	-8.62	0.51	-26.62	-7.19	-11.89	-7.93	0.39
80	-26.86	-5.67	-11.79	-9.69	0.29	-25.18	-5.09	-11.32	-8.95	0.17
81	-26.85	-10.06	-11.92	-5.02	0.16	-25.43	-9.34	-11.39	-4.71	-0.00
82	-25.35	-10.05	-4.19	-11.26	0.14	-23.97	-9.32	-3.92	-10.75	0.02
83	-17.38	0.41	-8.97	-8.95	0.14	-16.07	0.42	-8.31	-8.30	0.11
84	-30.08	-9.79	-8.59	-12.04	0.34	-28.35	-9.05	-7.94	-11.53	0.17
85	-26.41	-13.47	-4.21	-9.00	0.27	-24.93	-12.91	-3.90	-8.25	0.13
86	-31.53	-9.37	-12.66	-9.85	0.34	-29.76	-8.70	-12.12	-9.12	0.19
87	-28.61	-12.56	-11.12	-4.78	-0.15	-27.14	-11.99	-10.39	-4.49	-0.27
TAT (12)										
88	-39.08	-20.08	-0.70	-18.35	0.06	-38.01	-19.61	-0.70	-17.77	0.06
89	-35.11	-12.24	-2.91	-20.07	0.10	-33.98	-11.73	-2.70	-19.56	0.02
90	-38.48	-0.51	-16.67	-20.84	-0.46	-37.43	-0.53	-16.13	-20.32	-0.45
91	-32.85	0.77	-17.06	-16.86	0.30	-31.63	0.80	-16.43	-16.26	0.26
92	-32.57	-9.13	-6.68	-17.37	0.61	-31.06	-8.66	-6.01	-16.81	0.43
93	-23.06	-0.74	-11.47	-11.02	0.18	-21.42	-0.73	-10.63	-10.23	0.17
94	-22.07	-11.52	-10.11	-0.68	0.24	-20.65	-10.78	-9.40	-0.64	0.17
95	-35.95	-15.95	-10.80	-9.78	0.58	-34.23	-15.44	-9.96	-9.25	0.41
96	-35.50	-15.12	-10.11	-10.84	0.57	-33.78	-14.62	-9.57	-9.99	0.40
97	-34.18	-9.31	-9.10	-16.24	0.47	-32.57	-8.84	-8.33	-15.69	0.29

TABLE SIV: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
98	-32.27	-6.17	-9.73	-16.83	0.46	-30.61	-5.61	-9.07	-16.24	0.31
99	-33.33	-17.30	-10.00	-6.34	0.31	-31.67	-16.73	-9.39	-5.71	0.16
UUA (16)										
100	-38.95	-19.90	-0.73	-18.38	0.06	-37.88	-19.44	-0.72	-17.78	0.06
101	-37.84	-16.69	-20.32	-0.75	-0.08	-36.84	-16.19	-19.83	-0.75	-0.07
102	-38.21	0.03	-20.60	-17.15	-0.49	-37.05	0.03	-20.09	-16.50	-0.50
103	-38.37	-0.46	-16.72	-20.80	-0.41	-37.35	-0.47	-16.19	-20.28	-0.41
104	-37.80	-20.05	-0.71	-17.20	0.15	-36.71	-19.58	-0.70	-16.58	0.15
105	-35.74	-16.30	-17.15	-2.80	0.51	-34.49	-15.77	-16.56	-2.59	0.42
106	-32.94	-17.03	-17.08	0.85	0.32	-31.68	-16.41	-16.43	0.88	0.27
107	-32.81	-16.99	-16.79	0.68	0.30	-31.55	-16.37	-16.14	0.71	0.26
108	-29.97	-17.48	-9.59	-2.80	-0.10	-28.68	-16.83	-9.06	-2.58	-0.21
109	-29.16	-17.31	-2.54	-8.97	-0.34	-27.94	-16.69	-2.34	-8.44	-0.47
110	-30.87	-5.07	-18.03	-8.56	0.79	-29.44	-4.46	-17.48	-8.08	0.58
111	-20.18	-0.48	-10.35	-9.52	0.17	-18.70	-0.47	-9.56	-8.83	0.17
112	-19.55	-9.60	-0.31	-9.75	0.11	-18.12	-8.94	-0.28	-8.98	0.07
113	-35.35	-16.27	-9.28	-10.40	0.59	-33.67	-15.75	-8.77	-9.59	0.44
114	-34.58	-14.87	-10.43	-9.86	0.59	-32.91	-14.39	-9.62	-9.33	0.42
115	-32.82	-4.33	-9.61	-19.40	0.52	-31.34	-3.89	-8.92	-18.85	0.33
UUT (12)										
116	-37.50	-16.69	-0.87	-19.86	-0.08	-36.54	-16.20	-0.88	-19.40	-0.07
117	-37.36	-0.91	-16.56	-19.85	-0.04	-36.43	-0.92	-16.09	-19.39	-0.04
118	-35.51	-3.43	-12.11	-20.22	0.24	-34.42	-3.22	-11.61	-19.75	0.16
119	-35.46	-20.13	-3.53	-12.03	0.23	-34.39	-19.67	-3.33	-11.55	0.16
120	-32.72	-13.12	0.34	-19.94	-0.01	-31.83	-12.68	0.35	-19.48	-0.02
121	-17.41	0.53	-9.00	-8.93	-0.01	-16.20	0.54	-8.39	-8.32	-0.03
122	-16.99	-8.57	-8.95	0.50	0.04	-15.81	-7.98	-8.33	0.51	-0.00

TABLE SIV: (continued)

No.	without CP correction					with CP correction				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
123	-31.77	-9.39	-15.44	-7.68	0.74	-30.23	-8.90	-14.88	-7.03	0.57
124	-30.41	-6.50	-14.51	-10.18	0.79	-28.93	-5.88	-13.98	-9.67	0.60
125	-22.00	-6.62	-4.54	-10.70	-0.14	-20.57	-6.02	-4.00	-10.28	-0.27
126	-34.30	-11.26	-11.36	-11.34	-0.34	-32.78	-10.75	-10.83	-10.82	-0.39
127	-29.59	-6.46	-14.53	-9.12	0.52	-28.19	-6.09	-13.99	-8.52	0.41
UUU (14)										
128	-37.38	-19.78	-0.91	-16.64	-0.05	-36.43	-19.33	-0.91	-16.15	-0.04
129	-35.26	-11.89	-20.10	-3.45	0.18	-34.18	-11.40	-19.64	-3.24	0.10
130	-32.53	0.35	-19.82	-13.10	0.04	-31.65	0.35	-19.37	-12.66	0.02
131	-28.54	-15.23	0.01	-13.20	-0.13	-27.67	-14.79	0.02	-12.76	-0.14
132	-30.58	-16.79	-0.41	-13.10	-0.27	-29.66	-16.30	-0.41	-12.70	-0.25
133	-30.10	-6.17	-19.47	-5.05	0.59	-28.66	-5.71	-18.97	-4.39	0.41
134	-23.77	-13.57	-8.22	-1.85	-0.13	-22.53	-13.03	-7.73	-1.51	-0.26
135	-22.67	-12.77	-8.40	-1.55	0.05	-21.45	-12.23	-7.91	-1.25	-0.06
136	-16.85	-7.33	-9.29	-0.35	0.11	-15.61	-6.69	-8.67	-0.35	0.09
137	-30.41	-15.68	-6.25	-9.23	0.75	-28.93	-15.14	-5.64	-8.74	0.59
138	-30.27	-4.81	-19.02	-6.73	0.29	-28.87	-4.43	-18.50	-6.04	0.11
139	-28.50	-17.47	-8.29	-3.29	0.55	-27.06	-16.89	-7.62	-2.90	0.35
140	-29.68	-4.94	-7.35	-18.04	0.65	-28.32	-4.31	-6.93	-17.53	0.45
141	-34.42	-11.35	-11.35	-11.35	-0.37	-32.91	-10.83	-10.83	-10.83	-0.41

[a]grid m5. [b]grid 6. [c]grid 7.

TABLE SV: MP2/TZV(2df,2pd) fragmentation energies with CP correction and monomer relaxation (D_e), reference values from [1] (E_{ref}), and deviation ($D_e - E_{ref}$) in kcal mol^{-1} for DNA base trimers.

	ΔE	CPC	ΔE_{CPC}	E_{rel}	D_e	E_{ref}	Dev.
CCC (14)							
1	-52.86	-4.12	-48.73	6.65	-42.09	-41.55	-0.54
2	-52.27	-4.01	-48.26	5.98	-42.28	-41.28	-1.00
3	-50.30	-3.91	-46.39	5.60	-40.80	-39.67	-1.13
4	-50.20	-3.91	-46.29	6.07	-40.22	-38.55	-1.67
5	-46.32	-3.56	-42.76	4.89	-37.87	-36.24	-1.63
6	-38.82	-3.16	-35.65	4.28	-31.37	-29.50	-1.87
7	-51.39	-7.02	-44.37	6.50	-37.86	-37.70	-0.16
8	-49.96	-6.87	-43.09	6.66	-36.43	-36.67	0.24
9	-49.08	-6.47	-42.61	7.05	-35.55	-35.58	0.03
10	-47.21	-5.68	-41.53	6.45	-35.08	-35.08	-0.00
11	-47.73	-4.47	-43.26	5.41	-37.85	-37.79	-0.06
12	-36.08	-6.64	-29.44	4.05	-25.39	-26.01	0.62
13	-50.28	-6.35	-43.93	7.95	-35.99	-36.05	0.06
14	-41.49	-5.59	-35.90	3.17	-32.73	-31.72	-1.01
CGCplus (13)							
15	-85.59	-4.46	-81.13	10.19	-70.95	-73.68	2.73
16	-81.59	-3.74	-77.85	5.55	-72.30	-71.51	-0.79
17	-86.17	-4.53	-81.64	9.81	-71.83	-70.45	-1.38
18	-79.87	-3.62	-76.25	5.15	-71.11	-70.31	-0.80
19	-78.87	-3.55	-75.32	5.02	-70.30	-69.56	-0.74
20	-77.93	-3.45	-74.48	4.90	-69.58	-68.79	-0.79
21	-80.80	-3.72	-77.08	6.99	-70.09	-68.58	-1.51
22	-75.84	-3.44	-72.40	4.89	-67.51	-66.66	-0.85
23	-79.41	-7.84	-71.58	5.98	-65.59	-64.92	-0.67
24	-71.37	-6.56	-64.81	7.46	-57.34	-57.08	-0.26

TABLE SV: (continued)

	ΔE	CPC	ΔE_{CPC}	E_{rel}	D_e	E_{ref}	Dev.
25	-73.18	-3.72	-69.47	3.85	-65.61	-64.75	-0.86
26	-80.09	-7.72	-72.37	6.84	-65.53	-64.80	-0.73
27	-75.04	-7.00	-68.04	7.04	-61.00	-60.26	-0.74
GGG (12)							
28	-62.38	-3.78	-58.59	8.91	-49.68	-46.27	-3.41
29	-45.86	-3.41	-42.46	4.81	-37.65	-35.51	-2.14
30	-55.05	-4.90	-50.15	6.39	-43.76	-43.26	-0.50
31	-53.53	-4.87	-48.66	4.92	-43.74	-43.14	-0.60
32	-53.16	-4.87	-48.29	5.52	-42.77	-41.75	-1.02
33	-50.41	-4.44	-45.97	5.66	-40.31	-39.30	-1.01
34	-45.62	-3.93	-41.69	4.94	-36.76	-36.01	-0.75
35	-43.16	-10.38	-32.78	5.24	-27.54	-28.68	1.14
36	-62.39	-9.78	-52.61	6.99	-45.62	-44.81	-0.81
37	-58.88	-7.31	-51.57	6.41	-45.16	-44.42	-0.74
38	-58.16	-7.82	-50.34	17.84	-32.50	-47.39	14.89
39	-61.05	-5.68	-55.36	6.36	-49.00	-47.37	-1.63
mAmUmU (12)							
40	-35.02	-3.61	-31.41	3.36	-28.05	-27.82	-0.23
42	-35.53	-6.45	-29.08	1.71	-27.38	-27.06	-0.32
43	-37.45	-8.38	-29.07	1.96	-27.11	-27.53	0.42
44	-33.76	-7.58	-26.18	1.71	-24.47	-24.70	0.23
45	-43.88	-7.63	-36.25	2.93	-33.32	-33.08	-0.24
46	-43.33	-7.54	-35.80	3.06	-32.74	-32.36	-0.38
47	-42.92	-7.63	-35.29	2.95	-32.34	-32.11	-0.23
48	-43.26	-7.54	-35.72	3.42	-32.31	-31.95	-0.36
49	-43.57	-7.97	-35.59	3.30	-32.29	-31.93	-0.36
50	-37.49	-6.46	-31.03	2.10	-28.93	-28.72	-0.21
51	-35.67	-5.77	-29.90	2.43	-27.47	-27.31	-0.16

TABLE SV: (continued)

	ΔE	CPC	ΔE_{CPC}	E_{rel}	D_e	E_{ref}	Dev.
mCmCmC (12)							
52	-33.81	-3.19	-30.63	5.65	-24.97	-23.80	-1.17
53	-52.05	-8.10	-43.96	6.91	-37.05	-38.61	1.56
54	-51.99	-7.94	-44.05	6.88	-37.17	-36.09	-1.08
55	-22.14	-3.66	-18.48	0.71	-17.77	-17.34	-0.43
56	-40.43	-9.04	-31.39	3.32	-28.07	-28.12	0.05
57	-54.27	-8.05	-46.22	8.03	-38.19	-39.57	1.38
58	-52.41	-8.22	-44.19	8.48	-35.71	-38.60	2.89
59	-43.82	-6.53	-37.29	3.20	-34.10	-34.15	0.05
60	-44.40	-8.26	-36.13	3.68	-32.45	-32.95	0.50
61	-44.93	-8.28	-36.66	7.57	-29.09	-28.46	-0.63
62	-35.82	-6.02	-29.80	3.60	-26.20	-25.97	-0.23
63	-47.07	-7.17	-39.90	3.61	-36.30	-35.77	-0.53
mTmUmU (12)							
64	-24.65	-2.75	-21.90	1.81	-20.09	-20.13	0.04
65	-24.02	-2.71	-21.31	1.76	-19.54	-19.61	0.07
66	-32.64	-6.59	-26.05	2.01	-24.04	-24.07	0.03
67	-27.45	-3.76	-23.69	1.53	-22.17	-22.09	-0.08
68	-30.24	-6.85	-23.39	1.15	-22.24	-22.10	-0.14
69	-29.12	-7.10	-22.01	0.92	-21.09	-21.07	-0.02
70	-39.75	-7.26	-32.49	3.91	-28.58	-28.45	-0.13
71	-39.64	-7.20	-32.44	3.98	-28.46	-28.37	-0.09
72	-35.95	-6.60	-29.35	2.37	-26.98	-26.89	-0.09
73	-34.21	-6.76	-27.44	2.53	-24.91	-25.00	0.09
74	-29.73	-5.64	-24.10	1.71	-22.39	-22.28	-0.11
75	-38.71	-7.27	-31.45	3.81	-27.64	-27.56	-0.08
mUmUmU (12)							
76	-25.05	-2.89	-22.16	1.21	-20.95	-20.77	-0.18

TABLE SV: (continued)

	ΔE	CPC	ΔE_{CPC}	E_{rel}	D_e	E_{ref}	Dev.
77	-24.41	-2.71	-21.70	1.69	-20.00	-19.99	-0.01
78	-18.61	-2.31	-16.30	0.86	-15.45	-15.35	-0.10
79	-34.99	-6.40	-28.59	2.33	-26.26	-26.15	-0.11
80	-34.09	-6.44	-27.66	2.46	-25.19	-25.01	-0.18
81	-32.14	-5.33	-26.81	2.68	-24.13	-24.07	-0.06
82	-31.04	-5.31	-25.74	2.57	-23.17	-23.14	-0.03
83	-24.01	-6.20	-17.81	0.41	-17.40	-17.35	-0.05
84	-38.22	-7.12	-31.11	3.73	-27.37	-27.25	-0.12
85	-31.73	-5.63	-26.10	1.97	-24.13	-23.98	-0.15
86	-39.35	-7.12	-32.22	3.90	-28.33	-28.16	-0.17
87	-33.89	-5.71	-28.18	2.68	-25.50	-25.33	-0.17
TAT (12)							
88	-41.50	-3.45	-38.04	3.97	-34.07	-34.19	0.12
89	-38.50	-3.43	-35.07	3.29	-31.78	-31.85	0.07
90	-40.66	-3.29	-37.37	5.74	-31.63	-31.56	-0.07
91	-34.62	-3.50	-31.12	3.30	-27.82	-27.63	-0.19
92	-38.99	-5.77	-33.22	2.57	-30.66	-29.53	-1.13
93	-33.33	-7.92	-25.41	1.77	-23.64	-23.89	0.25
94	-30.71	-7.15	-23.56	2.70	-20.86	-21.13	0.27
95	-43.28	-7.03	-36.24	3.25	-32.99	-33.10	0.11
96	-42.98	-7.03	-35.95	3.27	-32.68	-32.81	0.13
97	-41.08	-6.35	-34.73	3.33	-31.40	-31.74	0.34
98	-40.21	-6.80	-33.41	3.15	-30.25	-30.41	0.16
99	-40.28	-6.33	-33.95	4.11	-29.83	-29.79	-0.04
UUA (16)							
100	-41.25	-3.42	-37.83	3.82	-34.00	-34.04	0.04
101	-39.99	-3.25	-36.74	3.44	-33.30	-33.36	0.06
102	-40.45	-3.45	-37.00	3.78	-33.22	-32.97	-0.25

TABLE SV: (continued)

	ΔE	CPC	ΔE_{CPC}	E_{rel}	D_e	E_{ref}	Dev.
103	-40.42	-3.24	-37.18	4.20	-32.98	-32.77	-0.21
104	-39.52	-3.50	-36.02	3.97	-32.05	-31.71	-0.34
105	-38.92	-3.63	-35.29	3.55	-31.73	-31.29	-0.44
106	-34.67	-3.57	-31.10	3.27	-27.83	-27.56	-0.27
107	-34.68	-3.59	-31.09	3.39	-27.69	-27.42	-0.27
108	-32.55	-3.38	-29.17	2.79	-26.39	-25.92	-0.47
109	-30.98	-3.32	-27.66	2.95	-24.71	-24.34	-0.37
110	-35.66	-5.27	-30.39	3.27	-27.12	-27.24	0.12
111	-29.41	-6.98	-22.43	1.16	-21.27	-21.44	0.17
112	-26.98	-6.52	-20.46	1.31	-19.15	-19.22	0.07
113	-42.30	-6.67	-35.63	3.19	-32.44	-32.51	0.07
114	-41.84	-6.72	-35.12	3.08	-32.04	-32.13	0.09
115	-39.22	-6.05	-33.17	2.65	-30.51	-30.73	0.22
UUT (12)							
116	-39.54	-3.26	-36.28	3.45	-32.82	-32.77	-0.05
117	-39.42	-3.23	-36.19	3.49	-32.71	-32.72	0.01
118	-38.84	-3.46	-35.38	3.43	-31.95	-31.84	-0.11
119	-38.74	-3.41	-35.32	3.41	-31.92	-31.82	-0.10
120	-34.62	-2.87	-31.75	2.70	-29.06	-28.99	-0.07
121	-23.70	-5.85	-17.85	2.16	-15.69	-15.78	0.09
122	-23.32	-5.72	-17.60	2.66	-14.93	-15.22	0.29
123	-38.16	-6.27	-31.89	2.88	-29.01	-28.87	-0.14
124	-36.58	-6.01	-30.58	2.76	-27.81	-27.65	-0.16
125	-27.12	-5.80	-21.32	1.51	-19.81	-19.76	-0.05
126	-38.65	-5.37	-33.28	4.63	-28.66	-28.87	0.21
127	-34.00	-4.98	-29.02	3.34	-25.68	-25.10	-0.58
UUU (14)							
128	-39.39	-3.24	-36.15	3.43	-32.72	-32.67	-0.05

TABLE SV: (continued)

	ΔE	CPC	ΔE_{CPC}	E_{rel}	D_e	E_{ref}	Dev.
129	-38.54	-3.41	-35.13	3.39	-31.74	-31.63	-0.11
130	-34.42	-2.85	-31.57	2.66	-28.91	-28.83	-0.08
131	-30.73	-2.76	-27.98	2.28	-25.70	-25.63	-0.07
132	-32.24	-2.87	-29.37	2.41	-26.96	-26.93	-0.03
133	-35.36	-5.57	-29.79	3.06	-26.73	-26.57	-0.16
134	-26.86	-3.74	-23.12	2.60	-20.52	-20.44	-0.08
135	-25.64	-3.40	-22.24	2.19	-20.05	-19.81	-0.24
136	-22.77	-5.61	-17.16	1.28	-15.88	-15.89	0.01
137	-36.52	-6.08	-30.44	2.83	-27.60	-27.56	-0.04
138	-34.93	-5.45	-29.48	2.51	-26.98	-26.96	-0.02
139	-33.80	-5.86	-27.94	2.42	-25.52	-25.62	0.10
140	-34.82	-5.14	-29.68	3.19	-26.48	-26.24	-0.24
141	-38.67	-5.32	-33.36	4.62	-28.74	-28.92	0.18

TABLE SVI: Contributions to the MP2/TZV(2df,2pd) interaction energies without CP correction (ΔE), two- (ΔE_{12}, ΔE_{23}, ΔE_{13}), and three-body terms (ΔE_3) in kcal mol^{-1} for DNA base trimers: exchange repulsion (EXR) and electrostatics (ES).

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
CCC (14)										
1	170.04	82.61	87.38	0.00	0.05	-172.54	-85.04	-89.55	2.05	-0.00
2	165.59	82.71	82.80	0.00	0.08	-168.33	-84.66	-84.96	1.29	-0.00
3	135.51	29.46	28.73	77.63	-0.31	-140.69	-27.83	-32.22	-80.64	0.00
4	159.93	88.12	71.77	0.00	0.05	-162.29	-90.11	-73.62	1.45	0.00
5	127.79	76.19	20.09	31.27	0.23	-132.38	-76.84	-22.49	-33.05	-0.00
6	111.70	90.63	21.02	0.00	0.05	-116.90	-91.82	-25.69	0.61	-0.00
7	156.67	78.60	32.69	45.55	-0.18	-153.00	-79.71	-31.11	-42.18	-0.00
8	161.18	49.67	22.31	89.69	-0.49	-155.82	-43.36	-21.27	-91.19	0.00
9	151.49	80.86	63.26	7.65	-0.29	-149.17	-82.76	-57.99	-8.43	0.00
10	145.26	0.10	83.59	61.49	0.08	-144.41	-0.14	-85.68	-58.59	-0.00
11	135.85	73.72	30.65	31.41	0.07	-139.94	-75.36	-30.75	-33.83	0.00
12	105.68	0.01	57.35	48.34	-0.01	-101.43	-0.09	-55.30	-46.04	-0.00
13	153.68	13.97	61.15	78.85	-0.29	-152.06	-17.04	-54.53	-80.49	0.00
14	108.55	33.24	36.57	38.78	-0.04	-107.75	-33.71	-37.00	-37.04	0.00
CGCplus (13)										
15	200.55	0.04	91.40	109.06	0.05	-211.30	3.75	-96.76	-118.29	0.00
16	161.39	0.00	56.03	105.10	0.26	-186.34	1.28	-69.94	-117.69	-0.00
17	195.33	94.29	94.63	6.62	-0.21	-208.05	-99.24	-104.52	-4.29	0.00
18	152.04	0.00	45.56	106.27	0.21	-178.94	0.45	-60.86	-118.53	0.00
19	144.31	0.00	45.33	98.62	0.36	-171.01	2.16	-60.19	-112.98	0.00
20	138.74	0.00	38.49	99.95	0.29	-165.99	3.90	-55.83	-114.05	0.00
21	161.15	0.00	79.04	81.83	0.28	-184.01	1.66	-94.22	-91.45	0.00
22	144.98	0.00	61.45	83.32	0.21	-168.69	0.77	-77.02	-92.44	-0.00
23	173.73	36.09	32.56	105.16	-0.08	-184.06	-23.43	-43.13	-117.50	-0.00

TABLE SVI: (continued)

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
24	177.46	56.91	0.06	120.42	0.08	-178.03	-53.09	4.78	-129.72	-0.00
25	124.91	21.60	28.42	74.58	0.31	-151.41	-18.38	-46.48	-86.55	0.00
26	170.71	29.10	39.05	102.60	-0.04	-182.92	-20.21	-47.22	-115.49	0.00
27	157.14	65.94	43.60	47.82	-0.22	-169.24	-65.03	-37.81	-66.40	0.00
GGG (12)										
28	130.04	43.37	43.36	43.35	-0.04	-148.68	-49.57	-49.56	-49.55	-0.00
29	113.25	57.67	55.54	0.00	0.04	-122.35	-62.29	-60.44	0.38	-0.00
30	170.63	0.00	91.39	79.24	0.01	-173.14	-1.31	-94.71	-77.13	0.00
31	132.18	29.14	57.64	45.51	-0.11	-136.68	-35.51	-57.25	-43.92	0.00
32	144.71	57.81	75.78	11.16	-0.03	-150.80	-60.64	-81.39	-8.78	-0.00
33	132.40	28.65	30.12	73.96	-0.33	-139.43	-30.57	-28.08	-80.78	0.00
34	125.37	36.01	0.00	89.33	0.02	-130.75	-37.25	-0.57	-92.92	-0.00
35	161.49	0.00	82.31	79.27	-0.10	-135.95	-0.08	-72.70	-63.16	-0.00
36	199.45	90.89	55.08	53.53	-0.06	-184.92	-92.67	-44.66	-47.59	0.00
37	152.07	49.11	38.16	65.02	-0.22	-152.42	-51.30	-42.63	-58.49	0.00
38	107.57	34.17	34.63	38.84	-0.08	-113.79	-43.41	-35.93	-34.46	0.00
39	133.12	44.38	44.34	44.36	0.04	-145.75	-48.60	-48.57	-48.58	-0.00
mAmUmU (12)										
40	131.42	67.53	0.00	63.92	-0.03	-127.50	-65.48	1.02	-63.04	-0.00
42	119.66	16.90	38.45	64.74	-0.43	-107.65	-14.63	-29.73	-63.28	0.00
43	126.05	67.66	0.00	58.48	-0.09	-106.43	-56.82	-0.50	-49.10	-0.00
44	115.67	0.00	46.60	69.09	-0.01	-97.90	0.26	-40.49	-57.67	0.00
45	146.93	56.20	32.13	58.70	-0.10	-135.35	-47.56	-31.35	-56.43	0.00
46	149.25	57.95	30.85	60.70	-0.26	-136.96	-48.04	-30.42	-58.50	0.00
47	146.10	60.52	27.48	58.30	-0.20	-133.48	-58.18	-26.29	-49.01	0.00

TABLE SVI: (continued)

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
48	147.53	58.96	29.11	59.84	-0.39	-135.12	-49.06	-28.23	-57.82	0.00
49	147.35	55.38	49.78	42.34	-0.15	-134.21	-46.77	-46.72	-40.72	0.00
50	127.94	67.09	4.75	56.31	-0.20	-115.26	-64.83	-5.64	-44.79	0.00
51	112.25	9.40	42.79	60.31	-0.26	-105.84	-9.02	-37.27	-59.55	-0.00
mCmCmC (12)										
52	103.21	13.51	0.03	89.63	0.05	-102.86	-15.08	0.67	-88.45	0.00
53	169.58	56.21	20.27	93.88	-0.78	-155.09	-47.48	-16.31	-91.30	0.00
54	163.98	87.56	18.82	58.39	-0.79	-151.72	-86.51	-15.97	-49.24	0.00
55	60.23	1.37	20.80	38.05	0.01	-59.12	-1.22	-20.78	-37.12	0.00
56	134.63	0.01	66.22	68.14	0.26	-115.53	-0.16	-56.93	-58.45	0.00
57	178.27	86.23	62.40	30.36	-0.71	-165.34	-84.42	-51.05	-29.87	0.00
58	174.79	62.70	93.11	19.88	-0.90	-161.34	-53.38	-89.17	-18.80	-0.00
59	120.22	47.54	39.36	33.70	-0.37	-116.34	-40.41	-41.16	-34.76	-0.00
60	148.83	38.81	53.70	56.38	-0.06	-132.76	-37.56	-48.71	-46.49	0.00
61	142.88	40.77	66.46	36.44	-0.80	-131.18	-39.67	-59.63	-31.88	0.00
62	98.38	50.67	28.14	19.77	-0.21	-94.12	-42.86	-28.44	-22.82	-0.00
63	134.19	45.94	43.41	44.81	0.03	-125.01	-43.30	-40.06	-41.65	0.00
mTmUmU (12)										
64	82.25	0.00	32.81	49.39	0.05	-82.32	0.06	-33.52	-48.86	-0.00
65	81.03	49.32	31.67	0.00	0.04	-80.72	-48.79	-31.89	-0.03	0.00
66	109.94	42.14	52.69	15.44	-0.33	-96.19	-33.07	-50.76	-12.36	0.00
67	80.58	49.21	18.03	13.34	-0.00	-80.16	-48.56	-17.05	-14.55	-0.00
68	92.00	0.00	44.77	47.27	-0.04	-79.29	0.50	-38.79	-41.00	-0.00
69	90.94	50.80	0.00	40.10	0.04	-75.09	-43.78	0.70	-32.01	0.00
70	132.40	40.04	35.21	57.04	0.11	-122.25	-33.67	-34.37	-54.22	0.00
71	132.05	56.56	38.86	36.51	0.12	-122.20	-53.84	-33.23	-35.14	0.00

TABLE SVI: (continued)

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
72	117.57	15.59	55.60	46.49	-0.12	-106.74	-14.01	-52.60	-40.12	0.00
73	112.15	39.41	51.27	21.65	-0.17	-99.20	-31.55	-49.60	-18.05	0.00
74	97.19	48.00	41.16	8.28	-0.25	-87.99	-47.39	-32.07	-8.53	-0.00
75	129.41	41.29	33.18	54.85	0.09	-118.66	-34.46	-31.59	-52.61	0.00
mUmUmU (12)										
76	68.98	42.71	10.97	15.25	0.05	-73.18	-43.52	-12.99	-16.67	-0.00
77	80.47	47.49	32.94	0.00	0.04	-80.83	-47.26	-33.61	0.04	-0.00
78	53.84	31.52	0.00	22.31	0.00	-55.57	-32.50	0.17	-23.24	-0.00
79	111.89	24.88	55.27	31.69	0.06	-103.89	-22.75	-53.02	-28.12	0.00
80	105.89	21.48	50.50	33.85	0.06	-99.38	-19.94	-49.59	-29.84	-0.00
81	100.48	46.31	46.52	7.77	-0.12	-95.17	-39.03	-46.05	-10.09	0.00
82	98.46	46.44	7.08	45.05	-0.11	-92.57	-39.16	-8.69	-44.73	0.00
83	79.94	0.00	39.88	40.09	-0.03	-65.71	1.18	-33.32	-33.57	0.00
84	126.24	39.85	33.13	53.18	0.09	-116.51	-33.73	-31.53	-51.24	0.00
85	102.71	52.01	9.73	41.25	-0.28	-94.41	-50.98	-10.15	-33.28	-0.00
86	129.86	35.65	55.56	38.54	0.11	-120.73	-34.74	-52.99	-33.00	0.00
87	108.05	53.91	42.27	11.86	0.01	-101.19	-51.34	-37.92	-11.94	0.00
TAT (12)										
88	136.94	66.50	0.00	70.30	0.14	-137.57	-68.39	-0.44	-68.74	0.00
89	119.89	54.10	3.86	61.77	0.17	-120.53	-52.08	-4.77	-63.68	0.00
90	133.78	0.00	59.30	74.52	-0.04	-132.56	-0.64	-58.32	-73.60	0.00
91	129.07	0.00	62.96	66.15	-0.03	-125.58	1.16	-62.45	-64.28	-0.00
92	126.53	29.55	38.55	59.07	-0.64	-120.45	-29.91	-31.40	-59.14	0.00
93	111.68	0.00	57.30	54.55	-0.17	-94.15	-0.16	-48.04	-45.95	-0.00
94	99.79	44.60	55.28	0.00	-0.09	-84.47	-38.72	-45.98	0.23	-0.00
95	139.98	58.94	42.69	38.53	-0.19	-131.39	-58.21	-36.32	-36.86	-0.00

TABLE SVI: (continued)

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
96	139.16	57.63	38.00	43.77	-0.23	-130.39	-57.03	-36.22	-37.14	-0.00
97	131.16	29.63	44.61	57.33	-0.41	-124.25	-29.66	-37.41	-57.17	-0.00
98	132.85	20.66	46.19	66.08	-0.08	-122.42	-19.01	-38.60	-64.81	-0.00
99	127.11	58.02	42.30	26.76	0.04	-121.45	-59.41	-39.14	-22.90	-0.00
UUA (16)										
100	133.91	65.32	0.00	68.45	0.14	-135.30	-67.48	-0.46	-67.36	-0.00
101	127.05	57.95	69.02	0.00	0.08	-128.35	-58.57	-68.95	-0.83	0.00
102	136.20	0.00	70.85	65.38	-0.03	-134.89	0.12	-70.67	-64.33	-0.00
103	132.11	0.00	58.29	73.86	-0.04	-131.25	-0.59	-57.58	-73.08	-0.00
104	135.12	65.55	0.00	69.42	0.15	-135.00	-67.74	-0.28	-66.98	0.00
105	126.53	62.06	61.49	2.78	0.20	-126.94	-61.35	-61.83	-3.76	0.00
106	129.31	67.02	62.32	0.00	-0.04	-125.71	-65.02	-61.94	1.25	0.00
107	132.23	65.91	66.36	0.00	-0.04	-128.07	-64.14	-65.00	1.07	0.00
108	105.67	65.56	33.35	6.70	0.05	-105.95	-64.69	-33.96	-7.30	0.00
109	107.78	68.44	3.16	36.19	-0.01	-105.62	-66.40	-3.82	-35.41	0.00
110	108.90	33.85	55.02	20.36	-0.34	-104.13	-25.85	-56.51	-21.77	0.00
111	98.59	0.00	50.59	48.13	-0.13	-83.64	-0.04	-42.82	-40.77	0.00
112	86.67	35.62	0.00	51.12	-0.07	-73.92	-31.45	0.39	-42.86	-0.00
113	135.38	58.07	36.29	41.20	-0.17	-128.81	-58.00	-35.05	-35.76	0.00
114	135.39	56.02	43.09	36.51	-0.23	-127.81	-55.71	-37.09	-35.01	0.00
115	130.51	14.03	45.36	71.36	-0.24	-119.53	-11.28	-38.55	-69.70	0.00
UUT (12)										
116	123.60	57.86	0.00	65.65	0.09	-127.17	-58.50	-1.04	-67.64	0.00
117	124.20	0.00	58.53	65.58	0.09	-127.52	-1.09	-58.86	-67.57	-0.00
118	116.58	6.58	49.15	60.73	0.11	-121.11	-8.06	-48.59	-64.47	-0.00
119	115.84	60.47	6.62	48.63	0.12	-120.50	-64.25	-8.08	-48.17	0.00
120	99.12	35.33	0.00	63.81	-0.02	-104.85	-38.99	0.48	-66.34	-0.00

TABLE SVI: (continued)

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
121	76.62	0.00	38.84	37.86	-0.08	-64.69	1.28	-33.41	-32.57	0.00
122	81.44	38.31	43.29	0.00	-0.16	-68.92	-33.58	-36.78	1.44	0.00
123	124.23	35.45	61.39	27.39	-0.01	-116.94	-35.30	-59.22	-22.41	-0.00
124	118.47	24.11	58.90	35.53	-0.06	-111.28	-19.02	-56.98	-35.28	0.00
125	87.58	34.84	19.89	32.99	-0.14	-77.21	-28.88	-14.29	-34.04	0.00
126	123.16	40.26	41.70	41.11	0.10	-121.85	-40.13	-41.15	-40.58	0.00
127	104.57	19.02	53.41	32.32	-0.19	-104.17	-20.14	-52.52	-31.50	0.00
UUU (14)										
128	123.22	65.26	0.00	57.87	0.09	-126.91	-67.31	-1.08	-58.52	0.00
129	115.32	48.72	59.88	6.60	0.11	-120.01	-48.11	-63.80	-8.11	-0.00
130	98.47	0.00	63.25	35.24	-0.02	-104.31	0.49	-65.89	-38.91	0.00
131	89.79	53.78	0.00	36.02	-0.01	-94.21	-54.70	0.05	-39.56	0.00
132	94.77	57.44	0.00	37.27	0.06	-99.28	-58.30	-0.49	-40.48	0.00
133	109.06	17.99	59.40	32.13	-0.45	-104.85	-18.25	-62.64	-23.97	-0.00
134	89.79	51.16	31.06	7.63	-0.06	-87.52	-50.86	-30.34	-6.32	0.00
135	85.60	49.66	30.42	5.49	0.04	-84.00	-49.11	-30.83	-4.06	-0.00
136	72.52	34.33	38.29	0.00	-0.09	-62.62	-28.58	-34.10	0.07	-0.00
137	118.41	60.46	23.21	34.78	-0.03	-111.56	-58.86	-18.17	-34.54	-0.00
138	107.37	10.01	63.96	33.55	-0.16	-102.43	-10.40	-65.29	-26.73	-0.00
139	112.12	65.73	35.72	10.78	-0.11	-103.12	-65.18	-29.90	-8.04	0.00
140	105.55	33.30	17.41	55.32	-0.49	-103.11	-25.12	-19.74	-58.25	-0.00
141	122.20	40.71	40.70	40.70	0.10	-121.49	-40.50	-40.50	-40.49	-0.00

TABLE SVII: Contributions to the MP2/TZV(2df,2pd) interaction energies without CP correction (ΔE), two- (ΔE_{12}, ΔE_{23}, ΔE_{13}), and three-body terms (ΔE_3) in kcal mol^{-1} for DNA base trimers: induction (Ind) and dispersion (Disp).

No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
CCC (14)										
1	-39.79	-19.05	-21.06	-0.10	0.43	-10.60	-5.51	-4.16	-0.77	-0.16
2	-37.87	-18.86	-19.00	-0.07	0.06	-11.89	-5.76	-5.63	-0.49	-0.01
3	-33.17	-6.14	-4.95	-17.85	-4.23	-11.94	-3.08	-3.40	-5.24	-0.23
4	-36.44	-21.19	-15.68	-0.04	0.47	-11.40	-4.17	-6.71	-0.37	-0.15
5	-29.05	-16.60	-4.24	-5.62	-2.59	-12.68	-6.73	-1.78	-3.82	-0.34
6	-26.21	-21.80	-4.43	-0.01	0.03	-7.42	-4.27	-2.79	-0.19	-0.17
7	-27.81	-17.15	-4.12	-5.91	-0.64	-27.24	-5.99	-9.12	-12.02	-0.11
8	-29.12	-5.65	-3.25	-21.72	1.50	-26.20	-15.28	-6.16	-4.34	-0.42
9	-24.93	-18.34	-6.48	-1.56	1.45	-26.45	-5.70	-17.76	-2.53	-0.46
10	-25.86	-0.26	-19.22	-7.28	0.89	-22.30	-0.52	-5.69	-15.80	-0.30
11	-31.04	-15.42	-5.77	-6.31	-3.53	-12.60	-6.10	-3.13	-3.21	-0.16
12	-11.47	-0.11	-6.68	-5.48	0.79	-28.86	-0.29	-14.90	-13.29	-0.38
13	-28.01	-3.11	-6.31	-18.60	0.01	-23.89	-2.27	-16.88	-4.43	-0.31
14	-22.25	-4.71	-6.54	-6.01	-5.00	-20.04	-6.55	-5.76	-7.59	-0.14
CGCplus (13)										
15	-59.83	-0.91	-21.15	-34.38	-3.39	-15.01	-0.37	-6.28	-7.69	-0.67
16	-44.60	-0.04	-17.95	-31.16	4.54	-12.03	-0.37	-4.03	-7.53	-0.11
17	-57.82	-21.80	-29.15	-0.94	-5.94	-15.63	-6.32	-7.46	-1.21	-0.64
18	-42.00	-0.04	-14.83	-31.39	4.26	-10.98	-0.17	-3.21	-7.58	-0.02
19	-39.34	-0.21	-14.24	-29.69	4.81	-12.86	-0.63	-5.07	-7.14	-0.02
20	-38.71	-0.19	-12.95	-30.04	4.47	-11.97	-1.14	-3.72	-7.17	0.06
21	-45.57	-0.04	-25.65	-24.80	4.93	-12.37	-0.44	-6.70	-5.08	-0.14
22	-40.77	-0.04	-20.24	-25.05	4.56	-11.36	-0.25	-5.91	-5.18	-0.02
23	-34.88	-2.97	-7.39	-30.90	6.38	-34.19	-18.63	-7.65	-7.67	-0.25

TABLE SVII: (continued)

No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
24	-43.46	-6.63	-1.58	-35.73	0.49	-27.34	-17.20	-1.73	-8.09	-0.31
25	-32.82	-3.84	-11.18	-22.94	5.14	-13.92	-4.39	-3.38	-6.04	-0.12
26	-34.09	-2.82	-7.80	-29.93	6.46	-33.79	-15.63	-10.22	-7.65	-0.30
27	-32.54	-14.65	-6.33	-15.70	4.14	-30.39	-6.84	-17.93	-5.61	-0.02
GGG (12)										
28	-35.75	-9.00	-9.00	-8.99	-8.76	-7.98	-2.47	-2.47	-2.47	-0.56
29	-25.97	-12.57	-12.19	-0.07	-1.14	-10.79	-5.22	-4.99	-0.23	-0.35
30	-37.18	-0.04	-21.37	-15.50	-0.28	-15.35	0.30	-6.47	-9.29	0.10
31	-33.14	-5.92	-11.85	-9.88	-5.49	-15.89	-3.32	-8.44	-3.91	-0.21
32	-32.42	-11.99	-17.82	-1.75	-0.87	-14.64	-5.66	-5.83	-3.07	-0.09
33	-29.00	-5.74	-4.20	-18.10	-0.96	-14.38	-4.92	-5.27	-4.11	-0.07
34	-28.51	-7.45	-0.01	-20.58	-0.47	-11.74	-4.96	0.09	-6.87	0.00
35	-12.68	-0.13	-6.28	-6.52	0.24	-56.02	-0.71	-27.31	-27.36	-0.64
36	-30.53	-20.17	-4.49	-6.67	0.79	-46.39	-7.90	-24.01	-14.35	-0.13
37	-28.66	-10.42	-7.84	-5.93	-4.47	-29.87	-6.19	-2.54	-20.78	-0.36
38	-20.91	-7.31	-7.32	-4.71	-1.57	-31.02	-8.32	-8.33	-14.10	-0.28
39	-32.28	-8.03	-8.02	-8.03	-8.21	-16.13	-5.23	-5.23	-5.23	-0.45
mAmUmU (12)										
40	-24.90	-12.99	-0.04	-12.07	0.20	-14.06	-6.79	-0.40	-6.88	0.01
42	-15.90	-1.47	-3.07	-11.98	0.62	-31.64	-7.06	-17.44	-7.16	0.01
43	-8.80	-5.16	-0.07	-4.11	0.53	-48.26	-24.83	-0.33	-22.55	-0.56
44	-8.66	-0.06	-3.69	-5.22	0.32	-42.87	-0.59	-16.54	-25.20	-0.54
45	-19.08	-4.21	-4.45	-10.27	-0.15	-36.39	-22.29	-6.56	-7.67	0.13
46	-19.29	-4.23	-4.33	-10.84	0.11	-36.33	-22.81	-5.98	-7.70	0.15
47	-18.95	-10.66	-4.00	-4.28	-0.00	-36.59	-7.63	-6.12	-23.01	0.16

TABLE SVII: (continued)

No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
48	-19.08	-4.43	-4.38	-10.62	0.36	-36.59	-23.32	-5.74	-7.68	0.15
49	-18.10	-4.18	-8.85	-5.19	0.13	-38.62	-22.39	-6.81	-9.35	-0.06
50	-17.41	-12.65	-0.85	-3.88	-0.04	-32.77	-7.41	-2.80	-22.73	0.18
51	-15.16	-1.23	-3.51	-10.66	0.25	-26.92	-4.09	-15.75	-7.13	0.04
mCmCmC (12)										
52	-20.68	-2.02	-0.04	-18.95	0.33	-13.49	-3.10	-0.35	-9.98	-0.06
53	-26.30	-5.53	-2.42	-19.75	1.40	-40.25	-20.85	-9.00	-10.35	-0.05
54	-25.34	-18.54	-2.36	-5.76	1.32	-38.90	-9.94	-7.68	-21.15	-0.14
55	-8.01	-0.14	-3.01	-4.90	0.04	-15.24	-0.85	-4.74	-9.63	-0.03
56	-12.46	-0.15	-6.33	-6.58	0.59	-47.06	-0.56	-22.76	-23.01	-0.73
57	-28.06	-18.20	-5.25	-5.29	0.67	-39.14	-9.71	-22.00	-7.11	-0.33
58	-26.64	-6.45	-19.55	-2.28	1.64	-39.22	-21.97	-10.38	-6.84	-0.03
59	-18.52	-3.69	-7.54	-6.33	-0.97	-29.18	-18.28	-4.94	-5.79	-0.17
60	-19.81	-7.04	-6.79	-4.57	-1.42	-40.66	-6.51	-13.30	-20.80	-0.04
61	-18.68	-5.43	-8.64	-5.12	0.50	-37.95	-11.46	-16.70	-9.69	-0.09
62	-12.55	-4.77	-4.80	-4.38	1.40	-27.52	-17.72	-6.87	-2.84	-0.09
63	-23.77	-7.26	-6.72	-5.37	-4.42	-32.48	-10.90	-9.55	-11.79	-0.24
mTmUmU (12)										
64	-15.60	-0.01	-6.08	-9.28	-0.22	-8.98	-0.12	-3.79	-5.05	-0.01
65	-15.23	-9.27	-5.71	-0.01	-0.24	-9.09	-5.04	-3.93	-0.11	-0.01
66	-14.41	-3.28	-9.90	-1.38	0.14	-31.98	-19.09	-5.60	-7.25	-0.05
67	-13.54	-9.29	-2.01	-2.03	-0.21	-14.33	-5.19	-6.89	-2.23	-0.03
68	-7.03	-0.07	-3.40	-4.04	0.47	-35.91	-0.57	-16.59	-18.31	-0.45
69	-6.83	-4.00	-0.04	-3.10	0.31	-38.14	-18.60	-0.57	-18.54	-0.43
70	-18.40	-3.40	-3.99	-11.08	0.07	-31.50	-16.47	-8.89	-6.03	-0.11
71	-18.30	-10.84	-3.38	-4.13	0.05	-31.20	-6.08	-15.48	-9.53	-0.10

TABLE SVII: (continued)

No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
72	-16.61	-1.92	-10.68	-3.82	-0.20	-30.17	-5.96	-6.26	-17.98	0.02
73	-14.99	-3.39	-9.54	-1.99	-0.08	-32.17	-17.71	-5.71	-8.77	0.02
74	-12.99	-8.91	-3.13	-1.26	0.31	-25.94	-5.40	-17.70	-2.73	-0.12
75	-17.39	-3.43	-3.81	-10.26	0.11	-32.08	-17.09	-8.91	-5.97	-0.10
mUmUmU (12)										
76	-12.11	-8.01	-2.04	-1.87	-0.19	-8.73	-4.65	-0.79	-3.25	-0.04
77	-15.19	-8.87	-6.10	-0.01	-0.21	-8.89	-4.96	-3.83	-0.12	0.02
78	-9.52	-5.83	-0.00	-3.67	-0.03	-7.36	-3.71	-0.06	-3.58	-0.00
79	-15.74	-2.38	-10.67	-2.99	0.29	-27.25	-9.55	-5.47	-12.09	-0.14
80	-14.61	-2.30	-9.39	-3.03	0.10	-26.00	-6.93	-5.14	-13.83	-0.09
81	-14.11	-3.77	-8.87	-1.58	0.11	-23.34	-16.79	-5.05	-1.37	-0.13
82	-13.14	-3.75	-1.31	-8.20	0.12	-23.79	-16.80	-1.71	-5.17	-0.11
83	-5.84	-0.05	-2.94	-3.02	0.17	-32.41	-0.70	-15.75	-15.62	-0.34
84	-16.95	-3.40	-3.76	-9.90	0.11	-31.00	-16.05	-9.03	-5.82	-0.11
85	-15.08	-10.51	-1.47	-3.38	0.27	-24.95	-5.13	-2.78	-16.99	-0.05
86	-18.07	-4.02	-10.75	-3.37	0.08	-30.41	-9.00	-5.90	-15.40	-0.11
87	-16.12	-10.37	-3.65	-1.77	-0.34	-24.63	-6.20	-15.18	-3.22	-0.02
TAT (12)										
88	-29.41	-14.85	-0.05	-14.40	-0.12	-11.46	-4.53	-0.20	-6.71	-0.02
89	-25.14	-10.62	-0.90	-13.36	-0.25	-12.73	-5.09	-1.36	-6.24	-0.04
90	-28.42	-0.01	-11.76	-16.16	-0.50	-13.46	0.15	-6.68	-6.98	0.05
91	-24.35	-0.05	-11.88	-12.64	0.22	-13.76	-0.44	-6.71	-6.62	0.01
92	-19.15	-5.39	-2.63	-12.07	0.93	-25.92	-4.47	-15.19	-6.31	0.06
93	-7.42	-0.06	-4.00	-3.70	0.33	-43.43	-0.42	-21.73	-20.84	-0.44
94	-6.99	-3.48	-3.71	-0.08	0.29	-39.05	-17.18	-20.78	-0.67	-0.42
95	-20.77	-12.43	-3.17	-5.71	0.53	-31.09	-5.30	-17.69	-8.16	0.07

TABLE SVII: (continued)

No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
96	-20.59	-11.95	-6.02	-3.23	0.61	-31.16	-5.28	-7.85	-18.07	0.05
97	-19.35	-5.57	-2.95	-11.48	0.65	-28.64	-4.46	-17.65	-6.49	-0.03
98	-18.10	-2.08	-3.49	-12.81	0.29	-32.54	-7.69	-18.02	-6.88	0.06
99	-18.62	-11.91	-5.04	-1.82	0.15	-27.31	-5.40	-10.99	-10.78	-0.14
UUA (16)										
100	-29.01	-14.72	-0.06	-14.12	-0.11	-10.85	-4.14	-0.19	-6.50	-0.02
101	-27.78	-12.58	-15.01	-0.02	-0.17	-10.90	-4.41	-6.60	0.07	0.04
102	-28.41	-0.01	-15.40	-12.44	-0.57	-13.36	-0.06	-6.66	-6.77	0.14
103	-28.23	-0.01	-11.68	-16.09	-0.45	-13.05	0.15	-6.47	-6.79	0.06
104	-28.39	-14.81	-0.08	-13.48	-0.03	-11.25	-4.14	-0.31	-6.71	-0.08
105	-26.27	-13.33	-12.34	-0.75	0.15	-12.23	-4.69	-6.17	-1.27	-0.10
106	-24.58	-12.92	-11.84	-0.05	0.23	-13.66	-6.61	-6.61	-0.46	0.02
107	-25.02	-12.69	-12.51	-0.04	0.22	-13.81	-6.56	-6.85	-0.40	0.01
108	-20.19	-12.62	-6.39	-0.92	-0.26	-12.06	-6.75	-3.56	-1.62	-0.12
109	-21.43	-13.39	-0.51	-7.02	-0.52	-11.70	-6.59	-1.37	-3.68	-0.07
110	-17.34	-2.70	-11.62	-3.65	0.63	-23.09	-12.89	-6.21	-4.15	0.16
111	-6.93	-0.05	-3.62	-3.53	0.27	-37.43	-0.32	-18.96	-17.79	-0.36
112	-6.03	-2.71	-0.06	-3.43	0.16	-33.70	-13.73	-0.52	-19.07	-0.37
113	-20.31	-12.48	-5.31	-3.08	0.56	-28.56	-4.80	-7.47	-16.32	0.03
114	-20.07	-11.68	-3.19	-5.83	0.62	-29.34	-5.00	-17.03	-7.36	0.04
115	-20.19	-1.66	-3.53	-15.29	0.28	-30.23	-6.10	-17.11	-7.38	0.35
UUT (12)										
116	-27.47	-12.56	-0.03	-14.70	-0.19	-8.49	-4.40	0.20	-4.31	0.02
117	-27.45	-0.03	-12.59	-14.68	-0.16	-8.65	0.22	-4.58	-4.32	0.03
118	-24.82	-1.47	-9.55	-13.76	-0.03	-9.45	-0.58	-4.84	-3.91	-0.12
119	-24.70	-13.77	-1.47	-9.41	-0.05	-9.38	-3.75	-0.71	-4.82	-0.11
120	-21.65	-7.27	-0.00	-14.35	-0.02	-7.25	-2.93	-0.14	-4.18	0.01

TABLE SVII: (continued)

No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
121	-4.99	-0.05	-2.52	-2.48	0.06	-30.64	-0.72	-14.96	-14.73	-0.23
122	-5.23	-2.60	-2.76	-0.06	0.19	-30.61	-13.49	-15.94	-0.87	-0.32
123	-20.06	-5.89	-12.76	-1.99	0.59	-25.54	-5.77	-6.01	-13.71	-0.05
124	-19.31	-1.70	-12.07	-6.26	0.72	-24.77	-12.87	-6.03	-5.87	0.01
125	-11.47	-2.62	-2.08	-6.50	-0.28	-26.03	-12.67	-9.48	-3.95	0.06
126	-20.70	-6.58	-6.82	-6.70	-0.61	-19.26	-6.22	-6.56	-6.59	0.11
127	-18.36	-3.36	-10.90	-4.50	0.41	-16.04	-3.10	-5.65	-7.34	0.06
UUU (14)										
128	-27.41	-14.67	-0.03	-12.55	-0.16	-8.29	-4.16	0.22	-4.39	0.03
129	-24.62	-9.41	-13.65	-1.48	-0.09	-9.23	-4.83	-3.71	-0.58	-0.10
130	-21.51	-0.00	-14.28	-7.24	0.02	-7.07	-0.15	-4.00	-2.93	0.02
131	-18.91	-11.32	-0.00	-7.44	-0.14	-7.40	-4.44	-0.02	-2.95	0.01
132	-20.48	-12.51	-0.01	-7.63	-0.33	-7.25	-4.32	0.10	-3.04	0.01
133	-18.01	-2.62	-13.33	-2.80	0.74	-21.56	-4.22	-4.02	-13.33	0.01
134	-17.30	-10.36	-5.80	-0.84	-0.30	-11.82	-4.61	-4.27	-2.87	-0.06
135	-16.46	-9.82	-5.79	-0.66	-0.19	-10.98	-4.76	-3.42	-2.80	0.01
136	-5.29	-2.71	-2.73	-0.04	0.20	-27.39	-13.35	-13.50	-0.31	-0.24
137	-19.52	-12.75	-1.64	-5.78	0.65	-23.84	-5.60	-12.51	-5.65	-0.09
138	-18.45	-1.58	-14.17	-2.83	0.13	-21.55	-3.17	-4.78	-13.89	0.29
139	-18.32	-13.93	-3.01	-1.81	0.43	-24.48	-5.64	-14.05	-4.92	0.13
140	-16.74	-2.62	-2.96	-12.01	0.84	-20.75	-13.20	-3.34	-4.34	0.12
141	-20.70	-6.69	-6.69	-6.69	-0.64	-18.69	-6.27	-6.27	-6.27	0.11

FIG. S1: Contributions (kcal mol^{-1}) to the B97-D/TZV(2df,2pd) TBE without CP correction vs. total MP2/TZV(2df,2pd) ΔE_3 with CP correction.

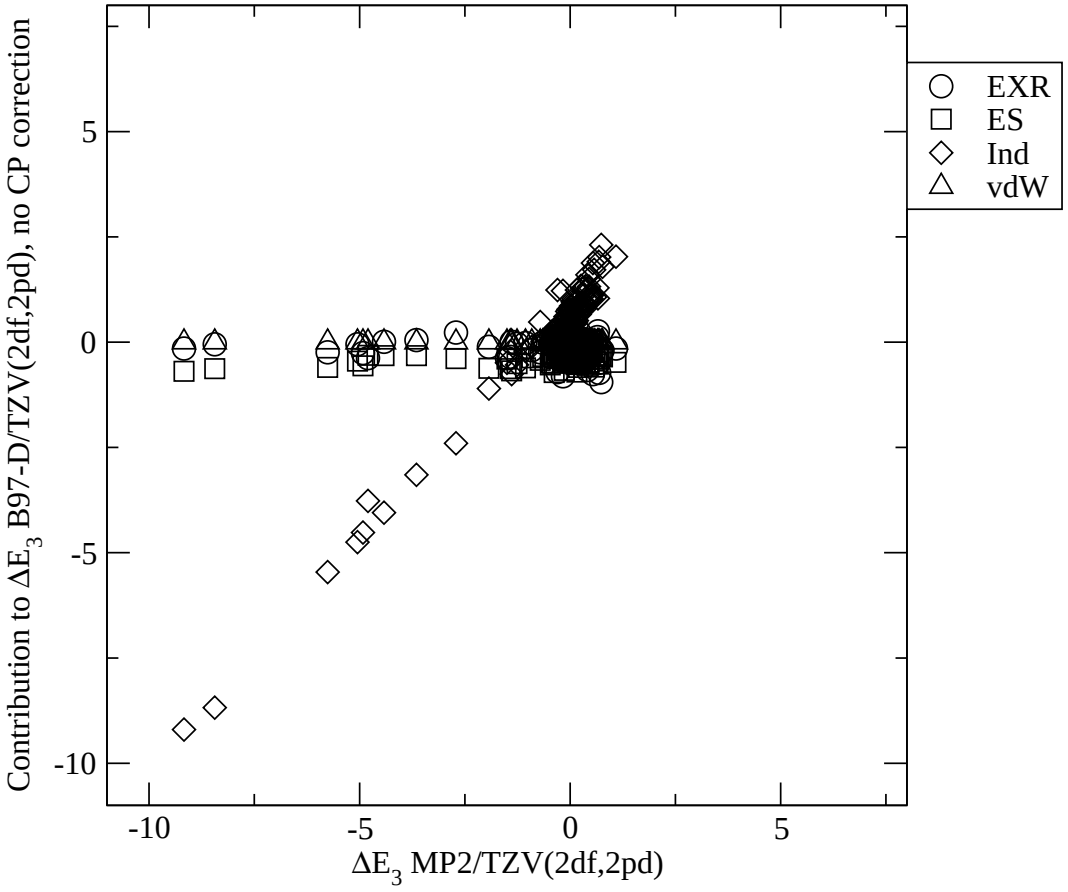


TABLE SVIII: Contributions to the B97-D/TZV(2df,2pd) interaction energies without CP correction (ΔE), two- (ΔE_{12}, ΔE_{23}, ΔE_{13}), and three-body terms (ΔE_3) in kcal mol^{-1} for DNA base trimers: exchange repulsion (EXR) and electrostatics (ES).

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
CCC (14)										
1	115.36	55.31	60.00	0.00	0.05	-104.03	-50.94	-54.39	1.66	-0.37
2	110.80	55.34	55.37	0.00	0.08	-100.54	-50.64	-50.76	1.30	-0.45
3	90.85	20.02	19.40	51.80	-0.38	-84.38	-16.20	-19.68	-48.19	-0.31
4	107.89	60.47	47.36	0.00	0.06	-98.06	-54.56	-44.48	1.49	-0.51
5	84.23	50.21	13.46	20.33	0.23	-79.27	-46.11	-13.66	-19.11	-0.39
6	76.39	62.15	14.18	0.00	0.06	-70.89	-55.43	-15.77	0.79	-0.48
7	100.15	52.32	19.35	28.66	-0.19	-83.18	-46.91	-15.55	-20.35	-0.37
8	103.67	29.30	13.32	61.54	-0.49	-85.16	-19.15	-10.60	-55.10	-0.31
9	96.19	54.12	37.73	4.54	-0.20	-81.87	-49.48	-28.59	-3.45	-0.35
10	93.50	0.08	55.95	37.35	0.12	-81.27	0.40	-51.17	-30.10	-0.40
11	89.30	48.45	20.38	20.41	0.05	-81.19	-44.12	-17.61	-19.13	-0.32
12	64.09	0.00	34.90	29.16	0.02	-50.86	0.30	-28.70	-22.07	-0.40
13	99.64	8.97	36.96	53.95	-0.24	-84.60	-9.43	-26.39	-48.35	-0.43
14	67.61	20.75	23.23	23.67	-0.05	-58.16	-18.26	-20.42	-19.03	-0.45
GGG (12)										
28	88.07	29.41	29.41	29.40	-0.15	-91.48	-30.27	-30.23	-30.29	-0.69
29	75.89	38.59	37.28	0.00	0.01	-74.45	-37.75	-36.73	0.71	-0.68
30	116.68	0.00	63.10	53.58	-0.00	-104.35	-0.62	-57.61	-45.45	-0.67
31	88.58	20.07	37.78	30.97	-0.24	-80.55	-21.81	-32.38	-25.75	-0.60
32	97.57	38.44	51.82	7.32	-0.02	-90.18	-36.03	-49.56	-3.98	-0.61
33	90.13	19.57	19.61	51.29	-0.35	-84.03	-17.96	-15.39	-50.06	-0.63
34	85.14	23.76	0.00	61.36	0.02	-78.92	-21.98	0.03	-56.26	-0.72
[a]	85.14	23.76	0.00	61.36	0.02	-79.89	-22.63	-0.64	-56.90	0.27
[b]	85.14	23.76	0.00	61.36	0.02	-79.62	-22.43	-0.46	-56.73	0.00
[c]	85.14	23.76	-0.00	61.35	0.03	-79.62	-22.43	-0.46	-56.73	0.00

TABLE SVIII: (continued)

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
35	94.80	0.00	48.63	46.23	-0.06	-60.19	0.44	-33.55	-26.38	-0.71
36	128.05	61.95	31.84	34.34	-0.07	-98.75	-55.35	-18.12	-24.69	-0.59
37	97.59	32.87	25.59	39.39	-0.26	-84.15	-30.36	-25.22	-28.01	-0.56
38	68.40	22.24	22.43	23.85	-0.11	-63.49	-25.82	-20.39	-16.66	-0.62
39	87.20	29.10	29.07	29.08	-0.05	-85.82	-28.39	-28.43	-28.38	-0.63
mAmUmU (12)										
40	87.87	45.41	0.00	42.50	-0.04	-75.65	-38.85	1.03	-37.31	-0.53
42	75.71	10.02	23.15	42.94	-0.40	-55.63	-5.75	-12.25	-37.39	-0.24
43	72.88	39.35	0.00	33.57	-0.04	-45.64	-24.56	-0.11	-20.41	-0.55
44	67.53	0.00	27.38	40.15	0.01	-42.76	0.71	-18.09	-24.78	-0.60
45	92.14	32.44	21.30	38.50	-0.10	-69.82	-20.21	-16.50	-32.69	-0.42
46	93.58	33.41	20.53	39.88	-0.24	-70.85	-20.31	-16.11	-33.94	-0.48
47	91.46	39.79	18.10	33.79	-0.21	-68.40	-33.62	-13.48	-20.89	-0.42
48	92.33	34.13	19.24	39.34	-0.39	-69.53	-20.89	-14.77	-33.43	-0.44
49	92.81	31.96	33.95	27.03	-0.14	-68.55	-19.91	-26.83	-21.36	-0.46
50	79.55	44.40	3.04	32.31	-0.21	-58.83	-38.01	-2.69	-17.77	-0.36
51	70.91	5.91	25.35	39.90	-0.25	-55.75	-3.71	-16.61	-35.05	-0.38
mCmCmC (12)										
52	67.58	8.74	0.02	58.75	0.06	-59.81	-7.75	0.83	-52.40	-0.48
53	105.98	33.32	11.84	61.55	-0.73	-81.07	-20.15	-6.83	-53.74	-0.35
54	101.97	57.40	11.07	34.26	-0.76	-79.23	-51.22	-7.16	-20.61	-0.24
55	38.77	0.88	13.22	24.63	0.03	-29.96	-0.07	-10.96	-18.43	-0.50
56	79.82	0.01	39.14	40.41	0.26	-50.82	0.26	-24.88	-25.68	-0.52
57	111.57	56.41	37.21	18.66	-0.71	-86.77	-49.79	-20.43	-16.16	-0.39
58	109.66	37.46	61.02	12.14	-0.95	-83.88	-23.20	-52.10	-8.26	-0.32
59	75.21	27.85	25.90	21.84	-0.38	-61.33	-16.65	-24.11	-20.17	-0.40
60	91.34	24.79	33.84	32.76	-0.04	-64.72	-20.79	-23.74	-19.68	-0.51

TABLE SVIII: (continued)

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
61	89.94	25.70	41.52	23.52	-0.81	-66.94	-21.10	-28.98	-16.60	-0.26
62	59.94	29.15	18.17	12.78	-0.15	-47.34	-17.84	-15.84	-13.18	-0.48
63	82.98	28.92	26.45	27.59	0.01	-64.40	-22.89	-20.32	-20.87	-0.32
mTmUmU (12)										
64	56.87	0.00	22.51	34.31	0.04	-49.27	0.27	-19.94	-29.20	-0.41
65	55.96	34.26	21.67	0.00	0.03	-48.18	-29.20	-18.77	0.15	-0.36
66	71.60	25.68	36.54	9.72	-0.34	-48.90	-13.73	-30.12	-4.77	-0.28
67	54.70	34.19	11.51	9.04	-0.04	-45.01	-28.97	-7.60	-8.10	-0.34
68	55.29	0.00	26.42	28.88	-0.01	-35.72	0.76	-17.24	-18.75	-0.50
69	54.44	30.07	0.00	24.32	0.05	-32.61	-19.65	0.76	-13.26	-0.45
70	86.72	23.88	23.07	39.66	0.10	-64.81	-14.74	-17.56	-32.15	-0.35
71	86.54	39.37	23.22	23.84	0.11	-64.95	-32.06	-14.70	-17.83	-0.36
72	76.61	10.53	38.57	27.66	-0.15	-55.93	-6.98	-31.12	-17.53	-0.30
73	73.19	24.02	35.48	13.86	-0.17	-50.36	-12.74	-29.40	-7.91	-0.32
74	63.02	33.21	24.68	5.38	-0.25	-45.25	-28.12	-13.21	-3.63	-0.29
75	84.64	24.76	21.86	37.95	0.08	-62.20	-15.03	-15.71	-31.09	-0.36
mUmUmU (12)										
76	47.49	29.80	7.51	10.14	0.05	-42.92	-26.23	-7.33	-8.97	-0.40
77	55.66	33.02	22.59	0.00	0.04	-48.38	-28.26	-19.96	0.29	-0.45
78	37.05	21.63	0.00	15.41	0.00	-32.79	-19.40	0.37	-13.32	-0.43
79	73.19	15.70	38.42	19.00	0.07	-54.77	-10.38	-31.65	-12.43	-0.32
80	70.03	13.64	35.00	21.35	0.05	-52.00	-8.93	-29.56	-13.24	-0.26
81	64.95	27.63	32.40	5.07	-0.15	-50.40	-17.04	-27.57	-5.49	-0.31
82	63.44	27.73	4.67	31.17	-0.13	-48.38	-17.10	-4.45	-26.51	-0.32
83	47.03	0.00	23.48	23.56	-0.01	-27.41	1.23	-13.99	-14.17	-0.48
84	82.61	23.96	21.79	36.80	0.07	-61.18	-14.96	-15.70	-30.34	-0.19
85	66.82	36.44	6.26	24.41	-0.29	-49.86	-30.86	-4.51	-14.19	-0.30

TABLE SVIII: (continued)

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
86	85.16	23.35	38.66	23.04	0.10	-64.26	-17.81	-31.53	-14.62	-0.31
87	70.53	37.51	25.00	8.06	-0.03	-54.20	-30.42	-17.08	-6.40	-0.30
TAT (12)										
88	93.11	45.47	0.00	47.49	0.15	-83.29	-41.56	-0.19	-41.10	-0.44
89	81.92	37.66	2.76	41.32	0.19	-72.38	-31.16	-2.08	-38.65	-0.48
90	88.89	0.00	39.02	49.91	-0.05	-79.70	-0.18	-34.81	-44.17	-0.54
91	86.45	0.00	41.96	44.53	-0.04	-74.80	1.20	-37.30	-38.21	-0.50
92	82.39	19.58	23.09	40.38	-0.66	-66.81	-16.91	-13.70	-35.88	-0.32
93	65.07	0.00	33.59	31.58	-0.11	-40.52	0.13	-20.93	-19.23	-0.49
94	59.22	27.40	31.89	0.00	-0.07	-36.57	-17.61	-18.98	0.52	-0.50
95	90.81	40.60	25.35	25.06	-0.21	-70.75	-34.98	-15.67	-19.62	-0.48
96	90.14	39.56	24.90	25.94	-0.26	-69.91	-34.00	-19.42	-15.99	-0.50
97	84.46	19.66	26.39	38.83	-0.43	-67.59	-16.74	-16.33	-34.09	-0.43
98	83.93	12.78	27.03	44.23	-0.11	-62.87	-8.38	-15.94	-38.19	-0.36
99	81.81	38.69	26.77	16.31	0.03	-65.25	-35.10	-20.05	-9.73	-0.38
UUA (16)										
100	91.01	44.67	0.00	46.20	0.14	-81.77	-40.86	-0.19	-40.30	-0.42
101	86.40	40.12	46.20	0.00	0.08	-77.99	-35.66	-41.56	-0.32	-0.45
102	90.85	0.00	47.37	43.51	-0.04	-80.87	0.32	-42.44	-38.25	-0.49
103	87.76	0.00	38.37	49.44	-0.05	-78.91	-0.15	-34.44	-43.82	-0.50
104	91.67	44.83	0.00	46.69	0.16	-81.20	-41.01	-0.06	-39.68	-0.46
105	86.52	43.00	41.26	2.04	0.22	-75.93	-37.08	-36.84	-1.64	-0.38
106	86.55	45.08	41.52	0.00	-0.05	-74.85	-38.61	-37.00	1.21	-0.45
107	88.45	44.37	44.12	0.00	-0.04	-76.05	-38.15	-38.48	1.02	-0.44
108	71.29	43.70	22.95	4.59	0.06	-63.19	-38.59	-20.22	-4.00	-0.38
109	73.12	46.01	2.21	24.91	-0.01	-62.72	-39.44	-2.03	-20.91	-0.34
110	70.71	20.84	36.77	13.41	-0.31	-56.93	-10.29	-34.02	-12.22	-0.40

TABLE SVIII: (continued)

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
111	57.02	0.00	29.34	27.76	-0.08	-35.79	0.20	-18.58	-16.92	-0.48
112	51.72	22.20	0.00	29.57	-0.05	-33.09	-14.88	0.69	-18.41	-0.49
113	87.98	40.03	23.63	24.51	-0.20	-70.10	-35.00	-18.77	-15.99	-0.34
114	87.70	38.52	25.52	23.92	-0.25	-68.99	-33.30	-16.48	-18.95	-0.26
115	82.76	9.33	25.99	47.70	-0.25	-62.50	-4.92	-15.86	-41.38	-0.34
UUT (12)										
116	85.06	40.07	0.00	44.90	0.09	-77.46	-35.55	-0.52	-40.99	-0.40
117	85.50	0.00	40.56	44.85	0.09	-77.74	-0.58	-35.77	-41.01	-0.38
118	80.46	4.59	34.15	41.59	0.13	-72.86	-4.24	-29.00	-39.24	-0.39
119	79.98	41.41	4.63	33.81	0.14	-72.65	-39.15	-4.37	-28.85	-0.28
120	67.50	23.85	0.00	43.67	-0.02	-63.49	-23.52	0.66	-40.17	-0.46
121	45.56	0.00	23.09	22.52	-0.05	-28.33	1.18	-14.78	-14.38	-0.36
122	48.34	22.58	25.86	0.00	-0.11	-30.45	-15.17	-16.25	1.36	-0.40
123	82.01	23.65	42.21	16.15	-0.00	-63.76	-19.11	-35.19	-9.17	-0.28
124	78.18	14.28	40.33	23.63	-0.07	-60.49	-7.43	-33.56	-19.25	-0.25
125	54.91	20.48	13.07	21.50	-0.13	-37.35	-11.96	-5.79	-19.40	-0.20
126	80.33	26.23	27.23	26.80	0.07	-69.05	-22.65	-23.25	-22.85	-0.29
127	70.69	13.09	36.62	21.17	-0.19	-59.44	-11.67	-31.26	-16.30	-0.21
UUU (14)										
128	84.80	44.63	0.00	40.08	0.09	-77.27	-40.78	-0.58	-35.55	-0.36
129	79.61	33.86	41.02	4.61	0.13	-72.32	-28.80	-38.94	-4.34	-0.23
130	67.06	0.00	43.29	23.79	-0.02	-63.13	0.63	-39.87	-23.47	-0.42
131	61.37	37.07	0.00	24.31	-0.01	-56.84	-32.88	0.26	-23.84	-0.39
132	64.95	39.76	0.00	25.12	0.07	-60.30	-35.50	-0.13	-24.34	-0.34
133	71.43	11.45	40.63	19.76	-0.40	-56.84	-9.47	-38.00	-9.09	-0.28
134	61.59	35.79	20.96	4.91	-0.07	-50.84	-30.92	-17.25	-2.36	-0.31
135	59.06	34.66	20.92	3.45	0.03	-49.16	-29.62	-18.19	-1.10	-0.25

TABLE SVIII: (continued)

No.	EXR					ES				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
136	43.78	21.09	22.76	0.00	-0.06	-27.94	-12.26	-15.63	0.28	-0.33
137	78.47	41.61	13.74	23.14	-0.03	-61.11	-35.10	-7.03	-18.73	-0.25
138	70.98	6.86	43.56	20.68	-0.13	-55.41	-5.11	-39.13	-10.89	-0.27
139	73.06	44.19	21.46	7.51	-0.10	-54.37	-38.15	-12.67	-3.30	-0.25
140	68.63	20.25	11.51	37.32	-0.45	-55.93	-9.80	-11.01	-34.90	-0.22
141	79.71	26.55	26.55	26.54	0.08	-68.98	-22.95	-22.88	-22.88	-0.28

[a]grid m5. [b]grid 6. [c]grid 7.

TABLE SIX: Contributions to the B97-D/TZV(2df,2pd) interaction energies without CP correction (ΔE), two- (ΔE_{12}, ΔE_{23}, ΔE_{13}), and three-body terms (ΔE_3) in kcal mol^{-1} for DNA base trimers: induction (Ind) and dispersion (Disp).

No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
CCC (14)										
1	-50.91	-24.46	-26.84	-0.35	0.73	-10.39	-5.71	-4.47	-0.22	0.00
2	-48.70	-24.34	-24.43	-0.37	0.45	-11.59	-5.67	-5.75	-0.16	0.00
3	-41.57	-8.15	-6.88	-22.78	-3.77	-11.51	-2.06	-3.70	-5.75	0.00
4	-47.43	-27.10	-20.83	-0.39	0.89	-10.29	-4.49	-5.70	-0.11	-0.00
5	-37.61	-21.89	-5.71	-7.60	-2.40	-10.94	-5.60	-1.53	-3.81	-0.00
6	-33.83	-27.80	-6.12	-0.32	0.42	-7.67	-4.52	-3.14	-0.01	-0.00
7	-35.74	-22.24	-5.67	-7.71	-0.11	-25.73	-6.20	-7.88	-11.65	-0.00
8	-37.40	-7.14	-4.41	-27.77	1.91	-23.86	-13.97	-5.28	-4.61	-0.00
9	-32.77	-23.79	-8.57	-2.19	1.79	-24.93	-5.62	-16.05	-3.26	-0.00
10	-33.80	-0.65	-24.82	-9.63	1.29	-20.73	-0.72	-5.71	-14.30	0.00
11	-39.14	-20.00	-7.89	-8.10	-3.15	-13.26	-6.28	-3.49	-3.49	0.00
12	-15.12	-0.40	-8.82	-6.96	1.07	-27.07	-0.48	-13.69	-12.90	0.00
13	-36.29	-4.31	-8.55	-23.91	0.48	-22.28	-2.71	-15.09	-4.49	0.00
14	-27.60	-6.34	-8.62	-7.89	-4.75	-17.70	-6.05	-5.15	-6.49	-0.00
GGG (12)										
28	-45.13	-11.98	-12.01	-11.95	-9.20	-9.39	-3.13	-3.13	-3.13	-0.00
29	-33.70	-16.46	-15.94	-0.54	-0.76	-11.07	-5.50	-5.41	-0.17	-0.00
30	-49.41	-0.49	-27.98	-21.44	0.51	-14.74	-0.07	-7.15	-7.52	0.00
31	-41.93	-8.30	-15.26	-12.91	-5.46	-15.60	-4.21	-8.01	-3.38	0.00
32	-42.61	-15.74	-23.33	-3.33	-0.21	-14.56	-5.56	-6.80	-2.21	0.00
33	-38.79	-8.13	-6.82	-23.62	-0.22	-14.34	-4.43	-4.34	-5.56	-0.00
34	-37.43	-10.19	-0.51	-27.03	0.30	-11.24	-3.79	-0.03	-7.43	0.00
[a]	-36.46	-9.54	0.16	-26.39	-0.69	-11.24	-3.79	-0.03	-7.43	0.00
[b]	-36.73	-9.73	-0.01	-26.56	-0.42	-11.24	-3.79	-0.03	-7.43	0.00
[c]	-36.73	-9.73	-0.01	-26.56	-0.42	-11.24	-3.79	-0.03	-7.43	0.00

TABLE SIX: (continued)

No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
35	-17.70	-0.64	-9.02	-9.00	0.96	-46.08	-0.79	-23.25	-22.04	0.00
36	-41.18	-26.51	-6.36	-10.02	1.72	-38.28	-8.01	-19.16	-11.11	-0.00
37	-37.47	-13.96	-10.34	-8.65	-4.52	-26.36	-5.84	-3.19	-17.34	0.00
38	-28.27	-10.06	-9.92	-7.19	-1.10	-29.11	-9.93	-7.62	-11.55	-0.00
39	-41.53	-10.98	-10.91	-10.97	-8.68	-17.20	-5.73	-5.73	-5.73	0.00
mAmUmU (12)										
40	-34.35	-18.21	-0.31	-16.67	0.83	-10.92	-5.52	-0.09	-5.31	0.00
42	-22.23	-2.39	-4.47	-16.66	1.30	-26.83	-7.20	-14.24	-5.38	0.00
43	-12.88	-7.55	-0.37	-5.97	1.01	-40.38	-20.78	-0.56	-19.04	0.00
44	-12.60	-0.54	-5.26	-7.68	0.88	-36.27	-0.69	-14.65	-20.93	0.00
45	-26.59	-6.12	-6.39	-14.68	0.60	-30.44	-18.50	-6.44	-5.50	0.00
46	-26.94	-6.30	-6.16	-15.44	0.96	-30.07	-18.52	-6.01	-5.54	-0.00
47	-26.33	-15.15	-5.73	-6.23	0.78	-30.56	-5.47	-6.01	-19.09	0.00
48	-26.43	-6.50	-6.10	-15.08	1.24	-30.50	-19.11	-5.78	-5.60	0.00
49	-25.56	-6.12	-12.69	-7.53	0.78	-32.32	-18.57	-5.38	-8.37	0.00
50	-24.04	-17.52	-1.45	-5.80	0.73	-27.49	-5.57	-3.25	-18.67	0.00
51	-21.19	-2.22	-4.92	-15.07	1.03	-24.20	-4.42	-14.29	-5.48	0.00
mCmCmC (12)										
52	-27.48	-2.89	-0.39	-25.01	0.81	-12.28	-3.98	-0.28	-8.02	0.00
53	-34.85	-7.51	-3.40	-25.96	2.02	-34.06	-18.00	-7.89	-8.16	0.00
54	-33.76	-24.50	-3.37	-7.77	1.88	-33.35	-7.96	-6.76	-18.64	0.00
55	-10.94	-0.67	-4.30	-6.59	0.62	-17.57	-1.19	-4.92	-11.46	-0.00
56	-16.48	-0.54	-8.41	-8.57	1.04	-41.53	-0.84	-20.24	-20.45	0.00
57	-37.41	-24.09	-7.39	-7.17	1.24	-34.80	-7.62	-21.40	-5.78	0.00
58	-35.41	-8.43	-25.87	-3.42	2.31	-35.54	-20.09	-7.91	-7.54	0.00
59	-24.44	-5.23	-10.14	-8.58	-0.49	-26.72	-17.32	-4.61	-4.79	0.00
60	-25.29	-9.33	-9.12	-6.31	-0.54	-37.03	-5.47	-13.06	-18.50	0.00

TABLE SIX: (continued)

No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
61	-24.78	-7.43	-11.39	-7.19	1.22	-34.10	-10.67	-15.32	-8.12	0.00
62	-17.20	-6.32	-7.05	-5.86	2.03	-25.22	-16.04	-6.42	-2.76	-0.00
63	-29.68	-9.56	-8.60	-7.48	-4.05	-28.75	-9.52	-8.43	-10.81	0.00
mTmUmU (12)										
64	-21.95	-0.27	-8.74	-13.10	0.16	-7.39	-0.08	-3.29	-4.02	0.00
65	-21.30	-13.03	-8.13	-0.23	0.09	-7.38	-4.02	-3.28	-0.08	-0.00
66	-20.57	-4.97	-13.98	-2.35	0.73	-27.34	-15.93	-4.29	-7.12	-0.00
67	-18.96	-13.19	-3.01	-3.02	0.26	-14.92	-4.11	-7.84	-2.96	0.00
68	-10.37	-0.41	-4.79	-6.06	0.89	-31.84	-0.54	-14.83	-16.47	0.00
69	-10.01	-5.66	-0.32	-4.75	0.72	-32.56	-16.61	-0.41	-15.54	-0.00
70	-25.86	-4.90	-5.85	-15.70	0.59	-27.82	-14.18	-8.97	-4.67	-0.00
71	-25.70	-15.36	-4.88	-6.05	0.58	-27.62	-4.71	-13.48	-9.43	0.00
72	-23.08	-3.02	-15.09	-5.36	0.38	-27.46	-6.20	-4.82	-16.45	0.00
73	-21.22	-5.05	-13.45	-3.25	0.52	-28.62	-15.42	-4.44	-8.76	-0.00
74	-18.52	-12.67	-4.69	-1.94	0.78	-22.52	-4.32	-14.66	-3.53	-0.00
75	-24.48	-5.05	-5.59	-14.46	0.62	-28.34	-14.65	-9.08	-4.61	-0.00
mUmUmU (12)										
76	-17.02	-11.49	-2.84	-2.98	0.30	-9.90	-3.83	-1.70	-4.37	0.00
77	-21.49	-12.62	-8.79	-0.30	0.22	-7.33	-3.96	-3.29	-0.08	-0.00
78	-13.64	-8.38	-0.25	-5.42	0.41	-6.75	-3.25	-0.01	-3.49	-0.00
79	-21.90	-3.54	-14.97	-4.15	0.76	-24.80	-9.55	-4.20	-11.04	-0.00
80	-20.45	-3.28	-13.17	-4.50	0.51	-24.44	-7.09	-4.06	-13.29	0.00
81	-19.68	-5.37	-12.67	-2.26	0.61	-21.71	-15.29	-4.08	-2.35	-0.00
82	-18.47	-5.36	-1.94	-11.76	0.59	-21.95	-15.32	-2.48	-4.15	-0.00
83	-8.44	-0.39	-4.30	-4.38	0.63	-28.56	-0.44	-14.16	-13.96	0.00
84	-23.88	-4.90	-5.46	-13.98	0.46	-27.63	-13.90	-9.22	-4.51	-0.00
85	-21.14	-14.90	-2.15	-4.95	0.86	-22.23	-4.14	-3.81	-14.28	-0.00

TABLE SIX: (continued)

No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
86	-25.36	-5.84	-15.21	-4.84	0.54	-27.08	-9.07	-4.58	-13.43	0.00
87	-22.25	-14.78	-4.91	-2.75	0.18	-22.68	-4.87	-14.12	-3.69	-0.00
TAT (12)										
88	-39.47	-19.77	-0.37	-19.68	0.35	-9.44	-4.23	-0.15	-5.07	0.00
89	-34.17	-14.76	-1.62	-18.20	0.40	-10.47	-3.98	-1.95	-4.54	-0.00
90	-38.26	-0.30	-16.37	-21.72	0.13	-9.41	-0.03	-4.50	-4.87	-0.00
91	-33.71	-0.33	-16.51	-17.71	0.84	-10.79	-0.10	-5.21	-5.47	0.00
92	-26.79	-7.49	-3.90	-16.99	1.60	-21.36	-4.31	-12.17	-4.88	0.00
93	-11.05	-0.33	-5.87	-5.62	0.77	-36.56	-0.54	-18.26	-17.76	0.00
94	-10.35	-5.27	-5.37	-0.52	0.80	-34.36	-16.03	-17.65	-0.68	-0.00
95	-28.77	-17.10	-4.80	-8.14	1.27	-27.24	-4.47	-15.69	-7.08	0.00
96	-28.52	-16.39	-8.61	-4.84	1.32	-27.22	-4.30	-6.98	-15.95	0.00
97	-27.07	-7.78	-4.49	-16.15	1.34	-23.98	-4.46	-14.68	-4.84	0.00
98	-24.74	-3.00	-5.01	-17.67	0.93	-28.59	-7.57	-15.81	-5.20	0.00
99	-25.61	-16.12	-7.12	-3.02	0.65	-24.28	-4.76	-9.60	-9.91	-0.00
UUA (16)										
100	-38.94	-19.55	-0.39	-19.32	0.33	-9.26	-4.16	-0.14	-4.96	0.00
101	-37.41	-17.12	-20.20	-0.38	0.29	-8.84	-4.03	-4.75	-0.06	0.00
102	-38.23	-0.25	-20.75	-17.27	0.04	-9.96	-0.04	-4.78	-5.14	-0.00
103	-37.92	-0.27	-16.20	-21.59	0.14	-9.30	-0.03	-4.45	-4.83	-0.00
104	-38.46	-19.69	-0.46	-18.76	0.45	-9.81	-4.17	-0.20	-5.44	-0.00
105	-35.70	-18.09	-16.89	-1.38	0.66	-10.64	-4.14	-4.69	-1.81	0.00
106	-33.98	-18.06	-16.45	-0.28	0.81	-10.65	-5.43	-5.14	-0.08	-0.00
107	-34.48	-17.79	-17.21	-0.26	0.78	-10.72	-5.42	-5.22	-0.08	0.00
108	-27.96	-17.42	-9.06	-1.70	0.22	-10.11	-5.18	-3.25	-1.68	0.00
109	-29.43	-18.57	-1.13	-9.73	0.01	-10.13	-5.30	-1.59	-3.24	0.00
110	-24.09	-3.81	-16.05	-5.73	1.50	-20.55	-11.81	-4.73	-4.02	0.00

TABLE SIX: (continued)

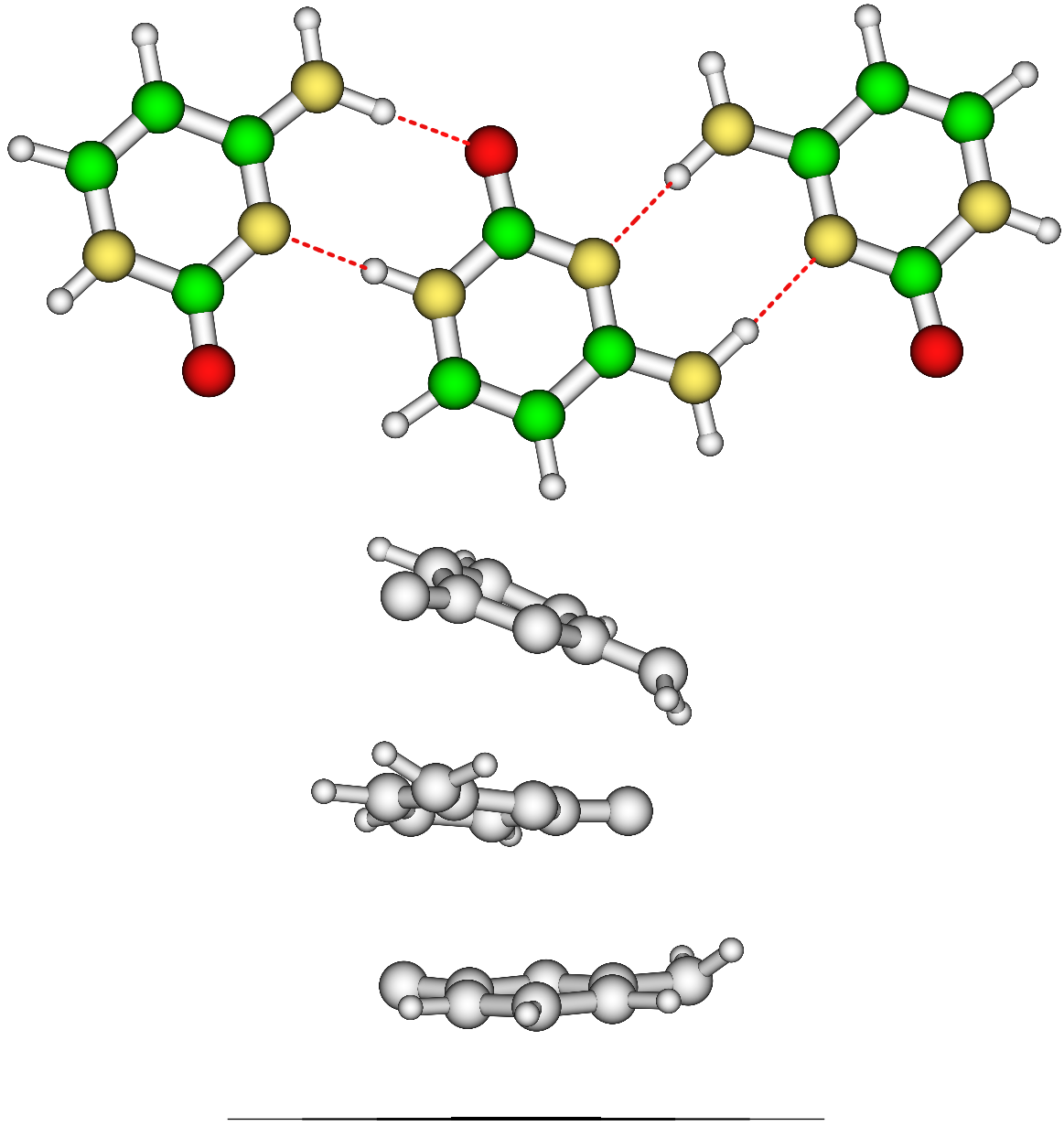
No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
111	-9.76	-0.30	-5.13	-5.06	0.74	-31.65	-0.38	-15.98	-15.30	-0.00
112	-8.94	-4.19	-0.46	-4.94	0.65	-29.24	-12.73	-0.54	-15.97	0.00
113	-27.95	-17.01	-7.55	-4.51	1.13	-25.28	-4.28	-6.59	-14.41	-0.00
114	-27.52	-15.91	-4.54	-8.18	1.10	-25.77	-4.18	-14.94	-6.65	0.00
115	-27.10	-2.65	-4.94	-20.62	1.11	-25.98	-6.09	-14.80	-5.09	-0.00
UUT (12)										
116	-36.83	-17.18	-0.30	-19.59	0.23	-8.27	-4.03	-0.06	-4.18	-0.00
117	-36.77	-0.28	-17.23	-19.51	0.25	-8.35	-0.05	-4.12	-4.18	0.00
118	-33.62	-2.18	-13.42	-18.53	0.51	-9.49	-1.61	-3.85	-4.04	0.00
119	-33.27	-18.37	-2.12	-13.16	0.38	-9.52	-4.01	-1.67	-3.83	0.00
120	-29.18	-10.07	-0.30	-19.29	0.48	-7.55	-3.39	-0.02	-4.14	0.00
121	-7.32	-0.29	-3.75	-3.69	0.40	-27.31	-0.37	-13.56	-13.38	-0.00
122	-7.65	-3.68	-4.16	-0.36	0.55	-27.21	-12.30	-14.41	-0.51	-0.00
123	-27.61	-8.02	-17.53	-3.07	1.02	-22.41	-5.91	-4.93	-11.58	-0.00
124	-26.53	-2.68	-16.53	-8.43	1.11	-21.56	-10.67	-4.75	-6.14	-0.00
125	-15.66	-3.70	-3.33	-8.82	0.18	-23.90	-11.44	-8.49	-3.97	0.00
126	-28.70	-9.33	-9.69	-9.55	-0.12	-16.89	-5.50	-5.65	-5.74	0.00
127	-25.45	-4.99	-15.06	-6.32	0.92	-15.40	-2.89	-4.83	-7.68	0.00
UUU (14)										
128	-36.68	-19.47	-0.27	-17.16	0.22	-8.23	-4.16	-0.05	-4.01	-0.00
129	-33.13	-13.13	-18.18	-2.11	0.29	-9.43	-3.82	-4.00	-1.61	0.00
130	-28.94	-0.26	-19.13	-10.03	0.49	-7.52	-0.02	-4.11	-3.39	-0.00
131	-25.74	-15.52	-0.23	-10.26	0.27	-7.33	-3.91	-0.02	-3.41	0.00
132	-27.75	-17.05	-0.25	-10.46	0.01	-7.48	-4.01	-0.04	-3.43	-0.00
133	-24.41	-3.79	-17.94	-3.96	1.27	-20.28	-4.37	-4.16	-11.75	-0.00
134	-23.96	-14.58	-8.24	-1.39	0.25	-10.56	-3.86	-3.70	-3.01	0.00
135	-22.79	-13.79	-8.09	-1.17	0.26	-9.79	-4.02	-3.03	-2.74	0.00

TABLE SIX: (continued)

No.	Ind					Disp				
	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3	ΔE	ΔE_{12}	ΔE_{23}	ΔE_{13}	ΔE_3
136	-7.63	-3.97	-3.88	-0.28	0.51	-25.06	-12.18	-12.53	-0.35	0.00
137	-26.80	-17.44	-2.54	-7.86	1.03	-20.97	-4.75	-10.43	-5.79	0.00
138	-24.77	-2.47	-18.94	-4.05	0.69	-21.07	-4.10	-4.50	-12.47	-0.00
139	-25.08	-18.64	-4.27	-3.07	0.90	-22.11	-4.87	-12.81	-4.44	-0.00
140	-22.72	-3.60	-4.29	-16.15	1.33	-19.66	-11.79	-3.56	-4.31	-0.00
141	-28.54	-9.42	-9.48	-9.47	-0.17	-16.61	-5.54	-5.54	-5.54	0.00

[a]grid m5. [b]grid 6. [c]grid 7.

FIG. S2: Structure of complex 12 (CCC S/S1) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.



[1] M. Kabelác, H. Valdes, E. C. Sherer, C. J. Cramer, and P. Hobza, Phys. Chem. Chem. Phys. **9**, 5000 (2007).

FIG. S3: Structure of complex 24 (CGCplus HB/S2) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.

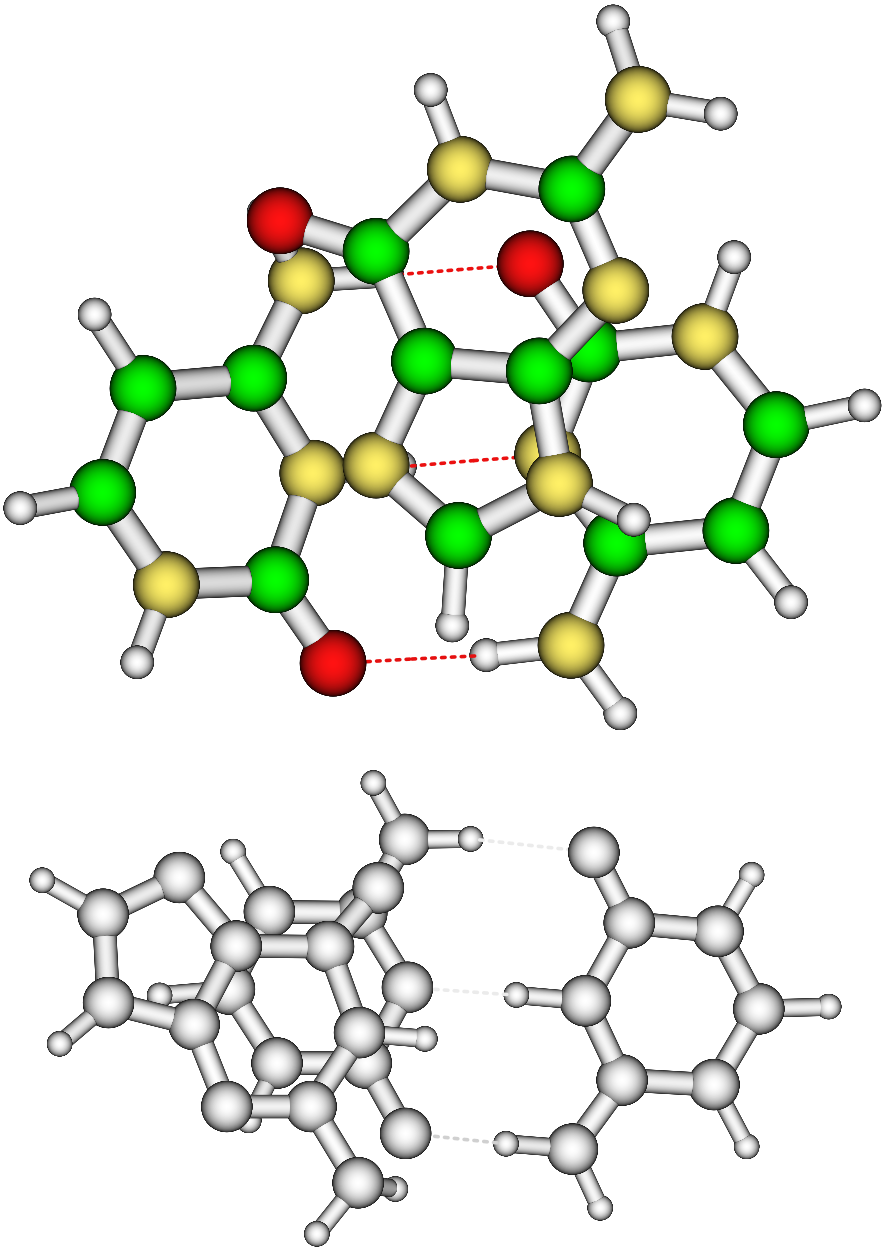


FIG. S4: Structure of complex 52 (mCmCmC HB/HB1) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.

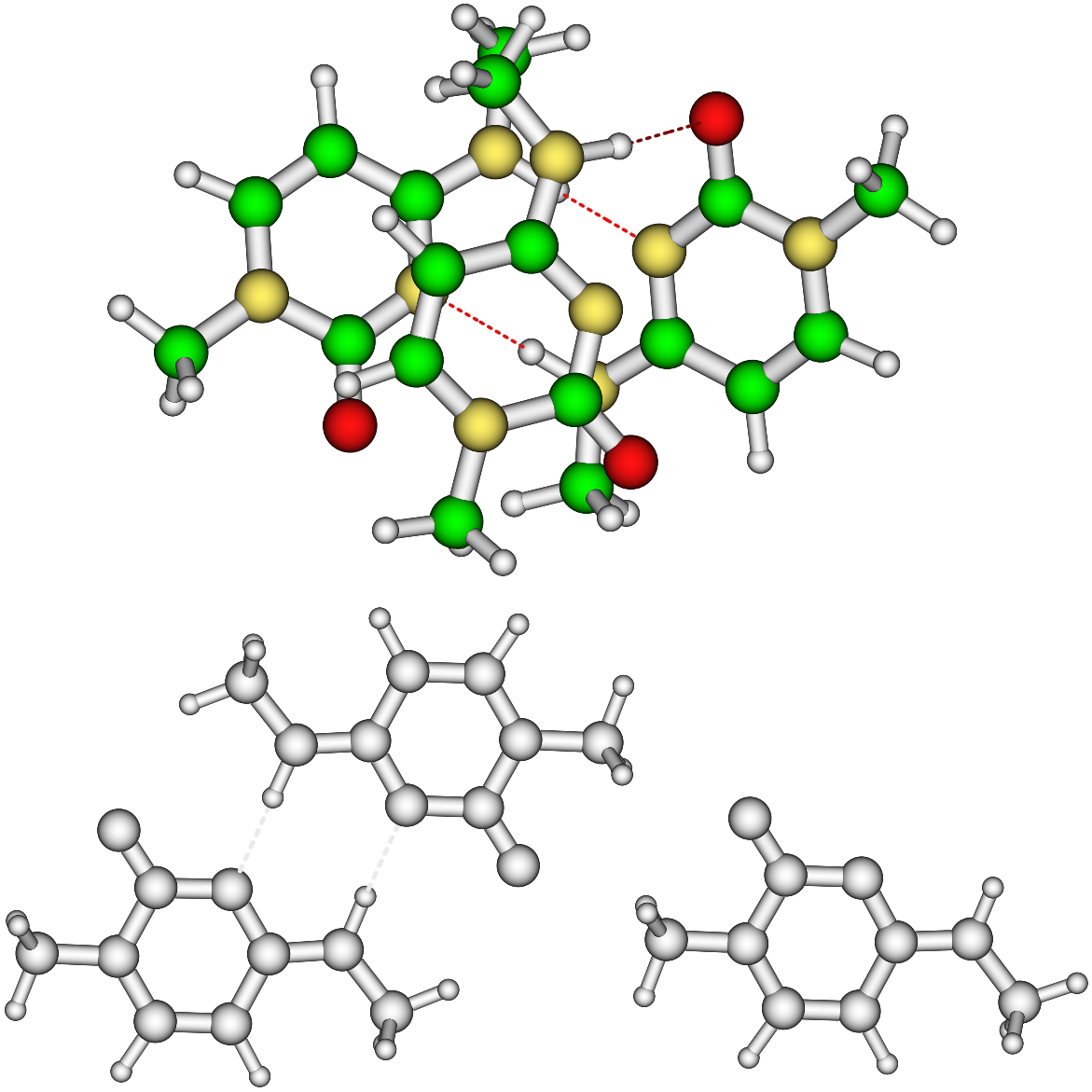


FIG. S5: Structure of complex 55 (mCmCmC HB/T1) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.

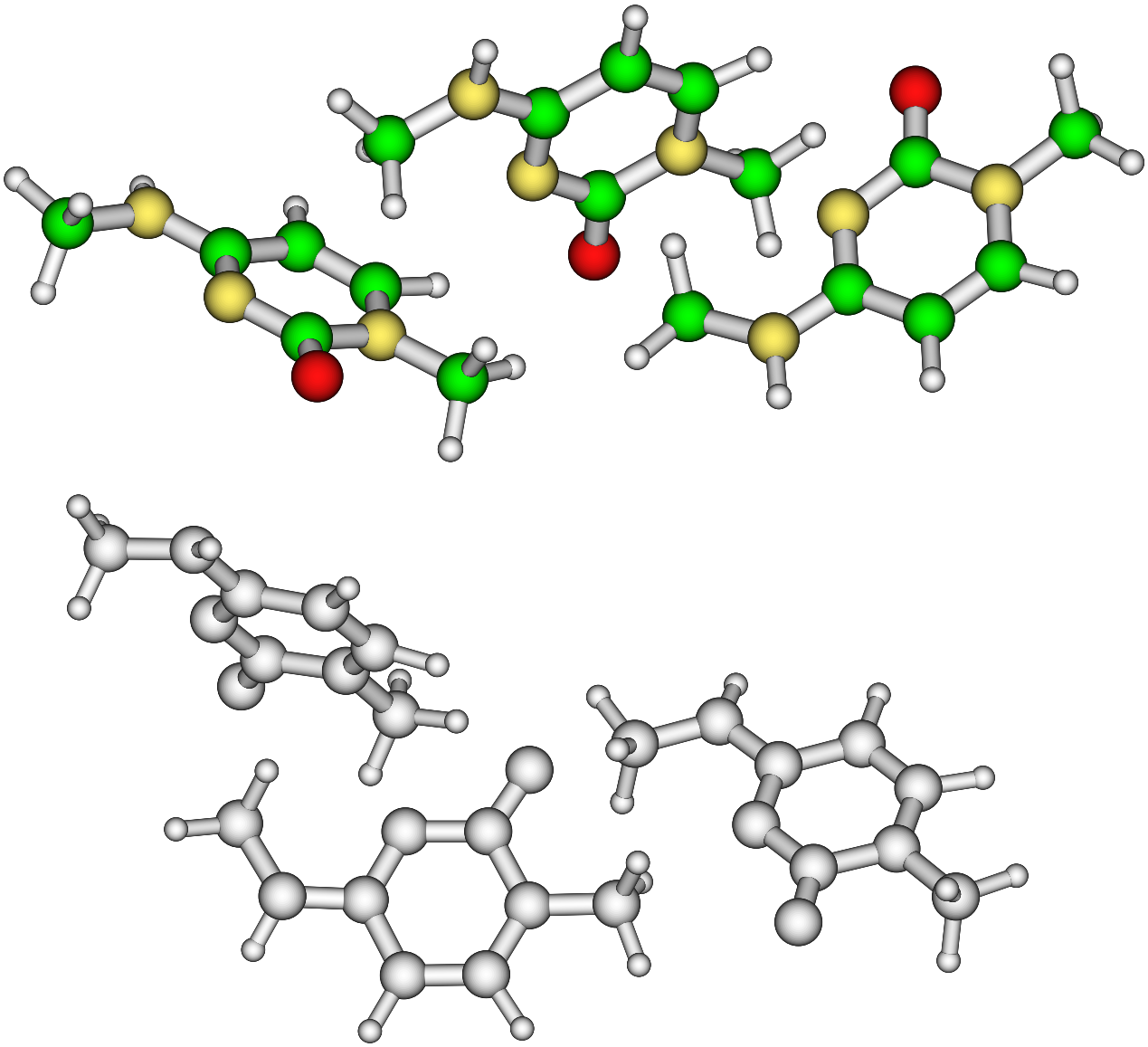


FIG. S6: Structure of complex 61 (mCmCmC S/T5) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.

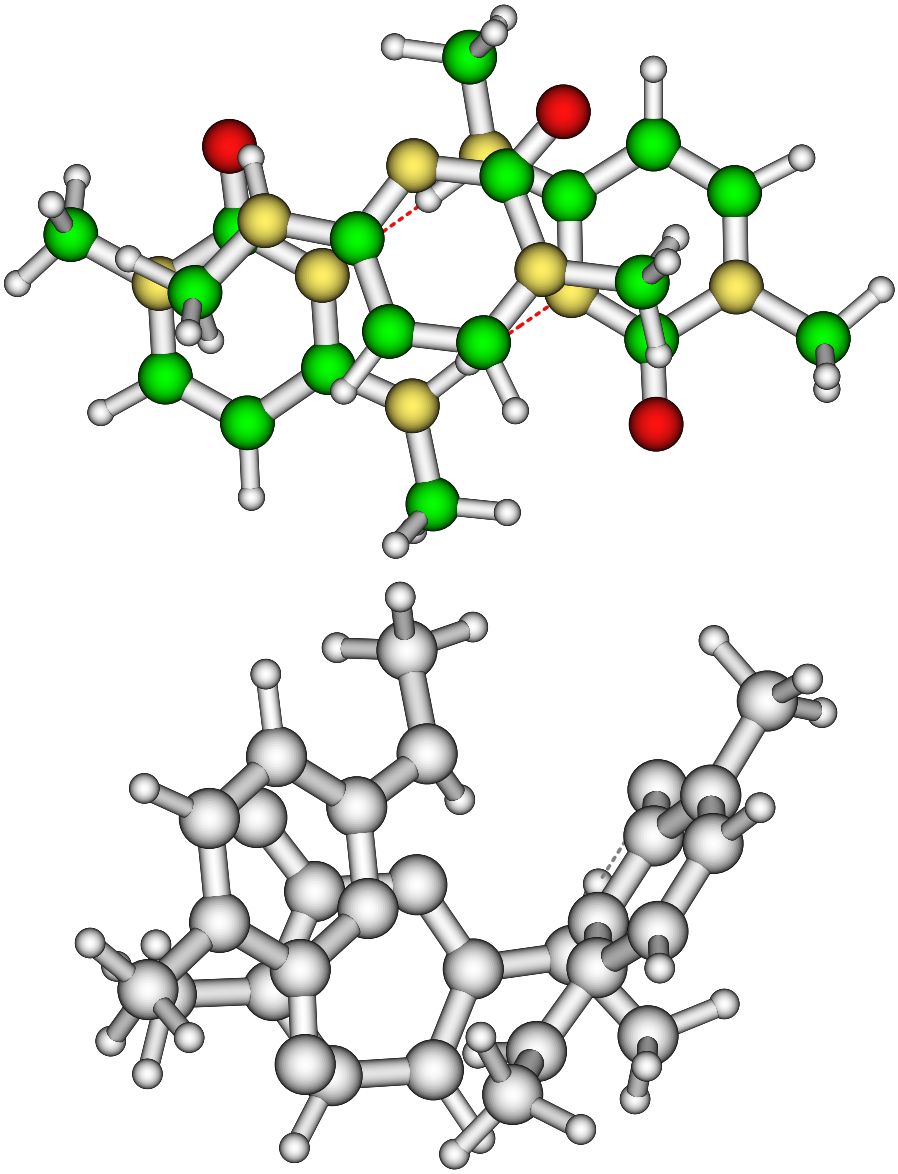


FIG. S7: Structure of complex 140 (UUU S/T4) before (bw) and after B97-D/TZV(2df,2pd) reoptimization.

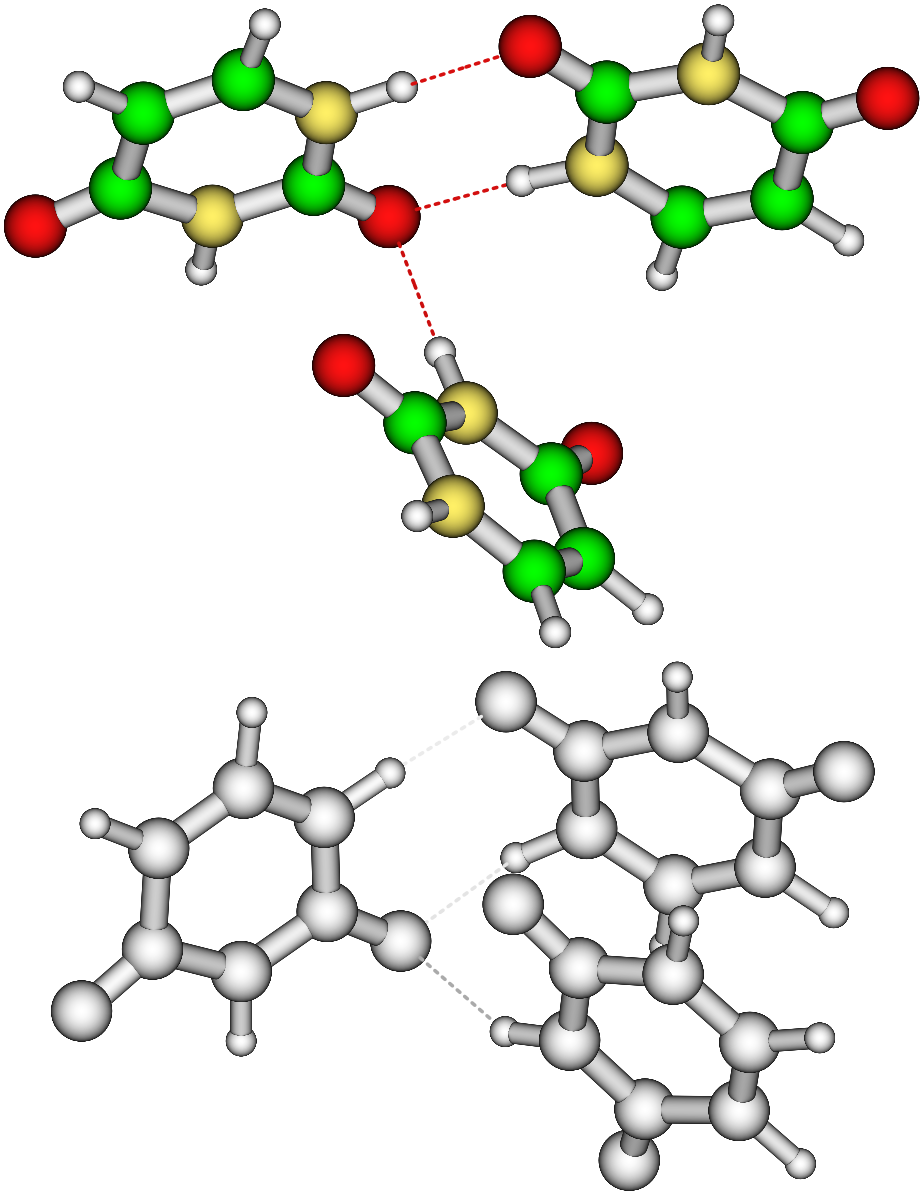


TABLE SX: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 12 (CCC S/S1).

N -0.2675076 -0.0231294 -6.5119158	C 1.0645280 -0.0176392 -6.7827289
H 1.3483682 -0.0239025 -7.8311693	C 1.9725711 -0.0050712 -5.7695914
H 3.0377897 -0.0006087 -5.9680202	C 1.4503601 0.0020266 -4.4241529
N 2.2779072 0.0144492 -3.3695130	H 1.9030577 0.0188077 -2.3980155
H 3.2730753 0.0184159 -3.5204032	N 0.1361138 -0.0036634 -4.1789350
C -0.7883501 -0.0157835 -5.1823200	O -2.0022577 -0.0207835 -5.0159916
H -0.9519903 -0.0318543 -7.2546335	N 0.4454494 -0.0294449 6.6772634
C 1.7811213 -0.0306987 6.4261297	H 2.4405231 -0.0462575 7.2894429
C 2.2365448 -0.0124817 5.1449089	H 3.2973399 -0.0129996 4.9233889
C 1.2432700 0.0065711 4.0954193	N 1.6193383 0.0257404 2.8101872
H 0.9075624 0.0300081 2.0487488	H 2.5969177 0.0213228 2.5709327
N -0.0686508 0.0062079 4.3607472	C -0.5408802 -0.0122931 5.6405850
O -1.7256011 -0.0147941 5.9531918	H 0.0903362 -0.0436536 7.6225004
N -0.8673000 0.0089179 -1.5391276	C -2.2026931 0.0010546 -1.3151775
H -2.8227427 -0.0085970 -2.2077422	C -2.6936494 0.0052444 -0.0423067
H -3.7592595 -0.0011173 0.1557235	C -1.7300113 0.0181187 1.0243039
N -2.1215037 0.0238260 2.3069286	H -1.4223043 0.0275359 3.0718714
H -3.1015571 0.0143073 2.5352192	N -0.4087113 0.0254194 0.7807081
C 0.0633206 0.0205385 -0.4925624	O 1.2832692 0.0257525 -0.7544404
H -0.5067668 0.0046238 -2.5192216	

TABLE SXI: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 24 (CGCplus HB/S2).

N 0.6374393 -3.4493335 0.8079472	H 0.6211705 -2.9356467 1.6940699
H 1.1609716 -4.3076019 0.7468437	C -0.0252030 -2.9897325 -0.2614845
C 0.0615757 -3.6835721 -1.5168529	H 0.6371658 -4.5950797 -1.6225260
C -0.6153438 -3.1496381 -2.5686604	H -0.6182845 -3.5889597 -3.5608494
N -1.3358879 -2.0091023 -2.4045129	H -1.8407766 -1.5960960 -3.1766495
C -1.4257840 -1.3375102 -1.1728677	N -0.7513605 -1.8678984 -0.1176329
O -2.1109213 -0.3071722 -1.1143651	C 0.1820081 2.5105270 -0.6301678
O -0.2953499 3.2974032 0.1810581	N -0.1114182 2.6752230 -2.0237254
H -0.6623861 3.4995894 -2.2319686	C 0.3058635 1.8579167 -3.0475404
N -0.0612320 2.2046241 -4.3111293	H 0.1895245 1.5696097 -5.0523334
H -0.8208566 2.8440704 -4.4770658	N 1.0630600 0.7937843 -2.8576690
C 1.4043771 0.6202965 -1.5636817	C 1.0304739 1.3682176 -0.4395596
N 1.5881499 0.8381881 0.7110194	C 2.2835430 -0.1938039 0.2986170
H 2.8610657 -0.8586369 0.9279293	N 2.2059293 -0.3777043 -1.0701544
H 2.6832498 -1.0739595 -1.6236860	N -2.1092698 1.2252632 1.1727178
H -2.1925687 0.5843936 0.3555489	H -2.3173779 2.2014121 1.0115038
C -1.2696258 0.9553460 2.1551680	N -0.7449652 -0.3012261 2.2366812
C 0.2120654 -0.6860881 3.1572744	H -0.8376627 -0.9437706 1.4007765
N 0.5094640 0.2749203 4.1152185	H 1.2021335 0.0080502 4.8019604
C -0.0067889 1.5393024 4.0957236	H 0.3473039 2.2108363 4.8701769
C -0.8991073 1.9144896 3.1442624	H -1.2851534 2.9230874 3.0941784
O 0.7527276 -1.7838191 3.1487651	

TABLE SXII: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 52 (mCmCmC HB/HB1).

C 2.4473819 2.4071993 0.4729038	H 2.5703668 2.5551130 -0.6031106
H 2.6623729 3.3515085 0.9931316	H 3.1530445 1.6373594 0.8106356
N 1.0738444 1.9827095 0.6945867	H 0.5135938 1.7514700 -0.1432046
C 0.6120506 1.5074212 1.8583971	C 1.4150754 1.4802842 3.0443750
H 2.4243513 1.8661542 3.0641669	C 0.8899421 0.8498430 4.1282855
H 1.4415347 0.7369311 5.0570500	N -0.3513974 0.2900792 4.1019524
C -0.8671422 -0.4817244 5.2313680	H -0.1952233 -0.3494161 6.0844930
H -1.8732604 -0.1361287 5.4856082	H -0.9270869 -1.5431923 4.9658999
C -1.1403825 0.3477837 2.9190973	O -2.2320927 -0.2459261 2.9031784
N -0.6475322 1.0355361 1.8666726	C -2.5151373 -2.5334926 -0.2203274
H -3.4093410 -2.4924183 0.4060913	H -2.6475327 -1.8467386 -1.0695398
H -2.4104779 -3.5540224 -0.6148133	N -1.3767265 -2.1659724 0.5971481
H -1.5706625 -1.7431880 1.4995826	C -0.1252163 -1.9840989 0.1070441
C 0.1626492 -2.2576020 -1.2712144	H -0.5761091 -2.6442607 -1.9605062
C 1.4170056 -1.9393479 -1.7036646	H 1.7197875 -2.0569504 -2.7402869
N 2.3491896 -1.4346070 -0.8660184	C 3.6566786 -1.0021696 -1.3567922
H 3.7845105 -1.3581555 -2.3832546	H 3.7115318 0.0906124 -1.3463888
H 4.4391652 -1.4062615 -0.7090208	C 2.0553575 -1.2397363 0.5358826
O 2.9530336 -0.8057458 1.2567095	N 0.7989109 -1.5405921 0.9578219
C -3.7381702 0.7191007 -0.1391358	H -3.8513915 0.5828010 0.9399408
H -4.3383800 1.5821267 -0.4641709	H -4.1198846 -0.1777167 -0.6449605
N -2.3256636 0.9175346 -0.3965301	H -1.6967698 1.0187102 0.4353038
C -1.7376180 0.8557341 -1.5950666	C -2.4705417 0.5309836 -2.7900257
H -3.5413934 0.3765693 -2.7876973	C -1.7530119 0.4163739 -3.9431970
H -2.2199384 0.1639931 -4.8919981	N -0.4088718 0.6060181 -3.9718324
C 0.3617482 0.4815616 -5.2070860	H -0.3173659 0.2233324 -6.0252371
H 0.8734395 1.4245611 -5.4246767	H 1.1260332 -0.2949399 -5.0957731
C 0.3054077 0.9750893 -2.7745300	O 1.5215629 1.1538417 -2.8583724
N -0.4156359 1.0972450 -1.6365357	

TABLE SXIII: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 55 (mCmCmC HB/T1).

O 2.6639506 0.7138355 4.0368121	C 1.6172557 0.1266895 4.2966524
N 0.8888753 0.3147766 5.4406093	C -0.2675897 -0.3122797 5.6096090
N -0.9631205 -0.0614728 6.7575946	C -0.4213970 0.7330223 7.8503537
H -1.2036583 0.8576182 8.6056917	H 0.4578099 0.2554798 8.3057548
H -0.1089087 1.7136719 7.4778471	H -1.7619516 -0.6442270 6.9457580
C -0.8267308 -1.2050766 4.6401361	H -1.7904145 -1.6831662 4.7778621
C -0.0918279 -1.4210557 3.5095389	H -0.4312972 -2.0466766 2.6899474
N 1.1081641 -0.8150630 3.3375774	C 1.8814591 -1.0151830 2.1135866
H 1.3398298 -1.7089833 1.4678081	H 2.0059637 -0.0546848 1.6047591
H 2.8761893 -1.3975874 2.3674713	O -1.7173229 0.1377193 -5.0291977
C -0.4861303 0.1346446 -5.0264619	N 0.2795775 0.0510537 -3.9033087
C 1.6065505 0.0649158 -3.9770682	N 2.3125272 0.0044823 -2.8234250
C 1.7048331 -0.1158701 -1.5014235	H 2.4719697 0.0874525 -0.7502974
H 0.8916841 0.6073894 -1.3995948	H 1.2942545 -1.1187878 -1.3334719
H 3.3156684 -0.0435002 -2.8936935	C 2.3112012 0.1503656 -5.2272522
H 3.3939508 0.1586255 -5.2834873	C 1.5488391 0.2236596 -6.3533472
H 1.9837426 0.2902641 -7.3468989	N 0.1911924 0.2193422 -6.2921936
C -0.6346478 0.2985551 -7.4976912	H 0.0196934 0.3556088 -8.3725831
H -1.2789518 -0.5837818 -7.5655502	H -1.2785374 1.1824960 -7.4497453
O -0.8066539 -2.1918775 0.3022055	C -1.1074515 -1.0296282 0.0108913
N -0.9410795 0.0283658 0.8538763	C -1.2550365 1.2613524 0.4656957
N -1.0882663 2.2741988 1.3548120	C -0.4997058 2.1086321 2.6804506
H -0.7372956 2.9937112 3.2777416	H -0.9211947 1.2218584 3.1598195
H 0.5902992 1.9909649 2.6354546	H -1.2406912 3.2101863 1.0166789
C -1.7545493 1.5518995 -0.8448951	H -1.9852327 2.5616635 -1.1664298
C -1.9206455 0.4937206 -1.6906953	H -2.2527292 0.6023149 -2.7178879
N -1.6373413 -0.7716406 -1.2905162	C -1.7842726 -1.9029906 -2.2084053
H -2.4829720 -2.6309026 -1.7829205	H -2.1387596 -1.5270166 -3.1698892
H -0.8156787 -2.3946439 -2.3380954	

TABLE SXIV: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 61 (mCmCmC S/T5).

O 3.1135474 0.8310469 1.8265470	C 3.0334383 -0.1636395 1.1042566
N 1.8761396 -0.6813598 0.6294580	C 1.8536567 -1.7272802 -0.2163014
N 0.6578802 -2.1502928 -0.6344811	C 0.4369718 -3.2484964 -1.5568686
C 3.0731589 -2.3549285 -0.6532921	C 4.2391990 -1.8684049 -0.1417809
N 4.2589530 -0.8200136 0.7198624	C 5.5099420 -0.2740484 1.2417377
H -0.1892205 -1.6790252 -0.2480817	H -0.6441668 -3.3410941 -1.6897528
H 0.9058417 -3.0550985 -2.5332361	H 0.8358104 -4.1956751 -1.1648941
H 3.0766065 -3.1943119 -1.3357742	H 5.2059735 -2.2922622 -0.4012053
H 6.3383439 -0.9097387 0.9149597	H 5.6567274 0.7491999 0.8781729
H 5.4695088 -0.2374565 2.3343396	O -2.8723861 -2.3564637 -0.9860202
C -2.8447568 -1.5688275 -0.0350605	N -1.7119577 -1.0244528 0.4695067
C -1.7312758 -0.1079536 1.4566104	N -0.5576944 0.3802248 1.8608462
C -0.3907415 1.4881984 2.7899235	C -2.9735724 0.3198521 2.0396776
C -4.1106489 -0.2584983 1.5692757	N -4.0857550 -1.1891570 0.5737200
C -5.3128095 -1.7719152 0.0354078	H 0.2898190 0.0374045 1.3805555
H 0.6826865 1.6636656 2.8886223	H -0.8692278 2.3936730 2.3967828
H -0.8098510 1.2431702 3.7760940	H -3.0129892 1.0848923 2.8021358
H -5.0938146 0.0038236 1.9502597	H -6.1598815 -1.4318405 0.6385717
H -5.4512105 -1.4677645 -1.0083064	H -5.2464621 -2.8638152 0.0605737
O -2.0397344 2.9730294 0.2245912	C -1.1980835 2.4258390 -0.4846848
N 0.1460355 2.5727264 -0.3482410	C 0.9914924 1.9575351 -1.1702415
N 2.3163612 2.1656422 -0.9448776	C 3.3711631 1.4663606 -1.6531346
C 0.5563308 1.1132868 -2.2425186	C -0.7902803 0.9254754 -2.3581913
N -1.6641697 1.5421116 -1.5310834	C -3.1043216 1.3292292 -1.6566460
H 2.5290531 2.5214976 -0.0221721	H 3.2672223 0.3738147 -1.5841300
H 3.3801322 1.7471601 -2.7146299	H 4.3285286 1.7568021 -1.2130158
H 1.2427334 0.5918030 -2.8960085	H -1.2213736 0.2590404 -3.1002112
H -3.2794540 0.4414563 -2.2710222	H -3.5269836 1.1873105 -0.6606787
H -3.5836235 2.2066027 -2.1076620	

TABLE SXV: Atomic coordinates (Å) of the B97-D/TZV(2df,2pd) reoptimized structure of complex 140 (UUU S/T4).

N 1.6015121 1.1239126 -0.6927158	C 2.6780542 0.4646179 -1.2369680
H 2.4256430 -0.2657695 -1.9986596	C 3.9483493 0.6969204 -0.8225994
H 4.7880804 0.1681185 -1.2544563	C 4.2086346 1.6661720 0.2297847
O 5.2900955 1.9736623 0.7029817	N 3.0183914 2.2841547 0.7218448
H 3.1405910 2.9642578 1.4626629	C 1.7233807 2.0542491 0.3174638
O 0.7542809 2.6330976 0.8225505	H 0.6457088 0.9266742 -1.0254306
N -0.2256736 -3.2027616 1.6736243	C 0.8019305 -4.0266444 1.2823447
H 1.0711219 -4.8036374 1.9913067	C 1.4299931 -3.8661470 0.0932258
H 2.2431166 -4.5118999 -0.2112681	C 1.0210751 -2.7935281 -0.8058827
O 1.5284373 -2.5312298 -1.8887604	N -0.0589532 -2.0213407 -0.3188341
H -0.3891304 -1.2520047 -0.9080374	C -0.7099038 -2.1447661 0.8957990
O -1.6142186 -1.4174446 1.2711591	H -0.6809039 -3.3267010 2.5658935
N -1.8390933 1.7921856 0.2105652	C -2.8884367 2.2134813 0.9882976
H -2.6180204 2.9146977 1.7714036	C -4.1581278 1.7832185 0.7899770
H -4.9770946 2.1210409 1.4116014	C -4.4452474 0.8342600 -0.2747281
O -5.5273692 0.3546377 -0.5659604	N -3.2833131 0.4748582 -1.0221587
H -3.4208808 -0.2022320 -1.7628857	C -1.9942283 0.8831356 -0.8038336
O -1.0401206 0.4689961 -1.4880385	H -0.8756667 2.1141097 0.4164334