Supporting Information

Dimer A, R = 4.0 A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	2.000000	-1.190336
2	6	0	1.233000	2.000000	-0.001136
3	6	0	-1.233000	2.000000	-0.001136
4	6	0	0.710208	2.000000	1.276436
5	6	0	-0.710208	2.000000	1.276436
6	1	0	2.272982	2.000000	-0.297918
7	1	0	-2.272982	2.000000	-0.297918
8	1	0	1.325261	2.000000	2.168811
9	1	0	-1.325261	2.000000	2.168811
10	16	0	0.000000	-2.000000	-1.190336
11	6	0	-1.233000	-2.000000	-0.001136
12	6	0	1.233000	-2.000000	-0.001136
13	6	0	-0.710208	-2.000000	1.276436
14	6	0	0.710208	-2.000000	1.276436
15	1	0	-2.272982	-2.000000	-0.297918
16	1	0	2.272982	-2.000000	-0.297918
17	1	0	-1.325261	-2.000000	2.168811
18	1	0	1.325261	-2.000000	2.168811

aug(d)-6-311G* basis set
E(RHF) = -1102.67966219
EUMP2 = -0.11040937575352D+04

6-31G* basis set
E(RHF) = -1102.57194178
EUMP2= -0.11038524311466D+04
CCSD(T)= -0.11039764664D+04

Dimer B, R = 4.0 A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.000000	1.189200	0.000000
2	6	0	-2.000000	0.000000	1.233000
3	6	0	-2.000000	0.000000	-1.233000
4	6	0	-2.000000	-1.277573	0.710208
5	6	0	-2.000000	-1.277573	-0.710208
6	1	0	-2.000000	0.296782	2.272982
7	1	0	-2.000000	0.296782	-2.272982
8	1	0	-2.000000	-2.169947	1.325261
9	1	0	-2.000000	-2.169947	-1.325261
10	16	0	2.000000	-1.189200	0.000000
11	6	0	2.000000	0.000000	1.233000
12	6	0	2.000000	0.000000	-1.233000

13	6	0	2.000000	1.277573	0.710208
14	6	0	2.000000	1.277573	-0.710208
15	1	0	2.000000	-0.296782	2.272982
16	1	0	2.000000	-0.296782	-2.272982
17	1	0	2.000000	2.169947	1.325261
18	1	0	2.000000	2.169947	-1.325261

aug(d)-6-311G* basis set
E(RHF) = -1102.68043519
EUMP2 = -0.11040941182696D+04

6-31G* basis set
E(RHF) = -1102.57276375
EUMP2= -0.11038530227068D+04
CCSD(T)= -0.11039771111D+04

Dimer C, R = 4.0 A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.842111	-0.156151	-1.413433
2	6	0	-0.444365	0.311767	-2.286270
3	6	0	-1.867386	1.318380	-0.541879
4	6	0	-0.008814	1.568568	-1.917149
5	6	0	-0.828474	2.148377	-0.912380
6	1	0	-0.015497	-0.355133	-3.021769
7	1	0	-2.638774	1.500514	0.193940
8	1	0	0.861056	2.046312	-2.352704
9	1	0	-0.668444	3.128245	-0.477788
10	16	0	1.842111	-1.301893	0.572059
11	6	0	0.444365	-1.823462	1.413937
12	6	0	1.867386	0.190531	1.412606
13	6	0	0.008814	-0.874994	2.317380
14	6	0	0.828474	0.285065	2.316613
15	1	0	0.015497	-2.793965	1.204562
16	1	0	2.638774	0.918744	1.202108
17	1	0	-0.861056	-1.013047	2.948957
18	1	0	0.668444	1.151645	2.947526

aug(d)-6-311G* basis set
E(RHF) = -1102.68027484
EUMP2 = -0.11040940978141D+04

6-31G* basis set
E(RHF) = -1102.57263194
EUMP2= -0.11038529146373D+04
CCSD(T)= -0.11039770017D+04

Dimer D, R = 4.8 A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	2.400568	-1.189768	.000000
2	6	0	2.400568	-.000568	1.233000
3	6	0	2.400568	-.000568	-1.233000
4	6	0	2.400568	1.277005	.710208
5	6	0	2.400568	1.277005	-.710208
6	1	0	2.400568	-.297350	2.272982
7	1	0	2.400568	-.297350	-2.272982
8	1	0	2.400568	2.169379	1.325261
9	1	0	2.400568	2.169379	-1.325261
10	16	0	-1.210232	-.000568	.000000
11	6	0	-2.399432	1.232432	.000000
12	6	0	-2.399432	-1.233568	.000000
13	6	0	-3.677005	.709639	.000000
14	6	0	-3.677005	-.710776	.000000
15	1	0	-2.102650	2.272414	.000000
16	1	0	-2.102650	-2.273550	.000000
17	1	0	-4.569379	1.324692	.000000
18	1	0	-4.569379	-1.325829	.000000

aug(d)-6-311G* basis set
E(RHF) = -1102.68156962
EUMP2 = -.11040935568403D+04

6-31G* basis set
E(RHF) = -1102.57390192
EUMP2= -0.11038533062280D+04
CCSD(T)= -0.11039777114D+04

Dimer E, R = 5.2 A
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	2.599432	-1.189768	.000000
2	6	0	2.599432	-.000568	1.233000
3	6	0	2.599432	-.000568	-1.233000
4	6	0	2.599432	1.277005	.710208
5	6	0	2.599432	1.277005	-.710208
6	1	0	2.599432	-.297350	2.272982
7	1	0	2.599432	-.297350	-2.272982
8	1	0	2.599432	2.169379	1.325261
9	1	0	2.599432	2.169379	-1.325261
10	16	0	-3.789768	-.000568	.000000
11	6	0	-2.600568	-1.233568	.000000
12	6	0	-2.600568	1.232432	.000000
13	6	0	-1.322995	-.710776	.000000
14	6	0	-1.322995	.709639	.000000
15	1	0	-2.897350	-2.273550	.000000
16	1	0	-2.897350	2.272414	.000000
17	1	0	-.430621	-1.325829	.000000
18	1	0	-.430621	1.324692	.000000

aug(d)-6-311G* basis set
E(RHF) = -1102.68286890
EUMP2 = -.11040932364791D+04

6-31G* basis set
E(RHF) = -1102.57535143
EUMP2= -0.11038538159074D+04
CCSD(T)= -0.11039785573D+04

Dimer F, R = 4.8 A
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.189768	-2.400568	.000000
2	6	0	-.000568	-2.400568	1.233000
3	6	0	-.000568	-2.400568	-1.233000
4	6	0	1.277005	-2.400568	.710208
5	6	0	1.277005	-2.400568	-.710208
6	1	0	-.297350	-2.400568	2.272982
7	1	0	-.297350	-2.400568	-2.272982
8	1	0	2.169379	-2.400568	1.325261
9	1	0	2.169379	-2.400568	-1.325261
10	16	0	-.000568	1.210232	.000000
11	6	0	-.000568	2.399432	1.233000
12	6	0	-.000568	2.399432	-1.233000
13	6	0	-.000568	3.677005	.710208
14	6	0	-.000568	3.677005	-.710208
15	1	0	-.000568	2.102650	2.272982
16	1	0	-.000568	2.102650	-2.272982
17	1	0	-.000568	4.569379	1.325261
18	1	0	-.000568	4.569379	-1.325261

aug(d)-6-311G* basis set
E(RHF) = -1102.68128913
EUMP2 = -.11040933733061D+04

6-31G* basis set
E(RHF) = -1102.57360036
EUMP2= -0.11038531008958D+04
CCSD(T)= -0.11039774427D+04

Dimer G, R = 5.2 A
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.189768	-2.599432	.000000
2	6	0	-.000568	-2.599432	1.233000
3	6	0	-.000568	-2.599432	-1.233000
4	6	0	1.277005	-2.599432	.710208
5	6	0	1.277005	-2.599432	-.710208

6	1	0	-.297350	-2.599432	2.272982
7	1	0	-.297350	-2.599432	-2.272982
8	1	0	2.169379	-2.599432	1.325261
9	1	0	2.169379	-2.599432	-1.325261
10	16	0	-.000568	3.789768	.000000
11	6	0	-.000568	2.600568	-1.233000
12	6	0	-.000568	2.600568	1.233000
13	6	0	-.000568	1.322995	-.710208
14	6	0	-.000568	1.322995	.710208
15	1	0	-.000568	2.897350	-2.272982
16	1	0	-.000568	2.897350	2.272982
17	1	0	-.000568	.430621	-1.325261
18	1	0	-.000568	.430621	1.325261

aug(d)-6-311G* basis set
E(RHF) = -1102.68306822
EUMP2 = -.11040934580054D+04

6-31G* basis set
E(RHF) = -1102.57573359
EUMP2= -0.11038540755703D+04
CCSD(T)= -0.11039787415D+04

Dimer H, R = 5.0 A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.190336	-2.500000	.000000
2	6	0	-.001136	-2.500000	1.233000
3	6	0	-.001136	-2.500000	-1.233000
4	6	0	1.276436	-2.500000	.710208
5	6	0	1.276436	-2.500000	-.710208
6	1	0	-.297918	-2.500000	2.272982
7	1	0	-.297918	-2.500000	-2.272982
8	1	0	2.168811	-2.500000	1.325261
9	1	0	2.168811	-2.500000	-1.325261
10	16	0	-1.190336	2.500000	.000000
11	6	0	-.001136	1.267000	.000000
12	6	0	-.001136	3.733000	.000000
13	6	0	1.276436	1.789792	.000000
14	6	0	1.276436	3.210208	.000000
15	1	0	-.297918	.227018	.000000
16	1	0	-.297918	4.772982	.000000
17	1	0	2.168811	1.174739	.000000
18	1	0	2.168811	3.825261	.000000

aug(d)-6-311G* basis set
E(RHF) = -1102.68339561
EUMP2 = -.11040938276928D+04

6-31G* basis set
E(RHF) = -1102.57554412
EUMP2= -0.11038540906745D+04

CCSD(T)= -0.11039787890D+04

Dimer I, R = 5.0 A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.500000	1.189200	.000000
2	6	0	-2.500000	.000000	1.233000
3	6	0	-2.500000	.000000	-1.233000
4	6	0	-2.500000	-1.277573	.710208
5	6	0	-2.500000	-1.277573	-.710208
6	1	0	-2.500000	.296782	2.272982
7	1	0	-2.500000	.296782	-2.272982
8	1	0	-2.500000	-2.169947	1.325261
9	1	0	-2.500000	-2.169947	-1.325261
10	16	0	2.500000	-1.189200	.000000
11	6	0	1.267000	.000000	.000000
12	6	0	3.733000	.000000	.000000
13	6	0	1.789792	1.277573	.000000
14	6	0	3.210208	1.277573	.000000
15	1	0	.227018	-.296782	.000000
16	1	0	4.772982	-.296782	.000000
17	1	0	1.174739	2.169947	.000000
18	1	0	3.825261	2.169947	.000000

aug(d)-6-311G* basis set
E(RHF) = -1102.68398144
EUMP2 = -.11040943238127D+04

6-31G* basis set
E(RHF) = -1102.57626267
EUMP2= -0.11038547987729D+04
CCSD(T)= -0.11039794499D+04

Dimer J, R = 5.0 A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.500000	.000059	-1.189768
2	6	0	-2.499691	1.233059	-.000568
3	6	0	-2.500309	-1.232941	-.000568
4	6	0	-2.499822	.710267	1.277005
5	6	0	-2.500178	-.710148	1.277005
6	1	0	-2.499430	2.273041	-.297350
7	1	0	-2.500570	-2.272923	-.297350
8	1	0	-2.499668	1.325320	2.169379
9	1	0	-2.500333	-1.325201	2.169379
10	16	0	2.499701	-1.190396	-.000568
11	6	0	1.267000	-.000886	-.000568
12	6	0	3.733000	-.001505	-.000568
13	6	0	1.790113	1.276555	-.000568

14	6	0	3.210528	1.276199	-.000568
15	1	0	.226943	-.297407	-.000568
16	1	0	4.772907	-.298547	-.000568
17	1	0	1.175284	2.169084	-.000568
18	1	0	3.825805	2.168419	-.000568

aug(d)-6-311G* basis set
E(RHF) = -1102.68364975
EUMP2 = -.11040940367918D+04

6-31G* basis set
E(RHF) = -1102.57584883
EUMP2= -0.11038543569766D+04
CCSD(T)= -0.11039789971D+04

Dimer K, R = 6.4 A
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	0.000000	-2.009664
2	6	0	0.000000	1.233000	-3.198864
3	6	0	0.000000	-1.233000	-3.198864
4	6	0	0.000000	0.710208	-4.476436
5	6	0	0.000000	-0.710208	-4.476436
6	1	0	0.000000	2.272982	-2.902082
7	1	0	0.000000	-2.272982	-2.902082
8	1	0	0.000000	1.325261	-5.368811
9	1	0	0.000000	-1.325261	-5.368811
10	16	0	0.000000	0.000000	4.390336
11	6	0	0.000000	1.233000	3.201136
12	6	0	0.000000	-1.233000	3.201136
13	6	0	0.000000	0.710208	1.923564
14	6	0	0.000000	-0.710208	1.923564
15	1	0	0.000000	2.272982	3.497918
16	1	0	0.000000	-2.272982	3.497918
17	1	0	0.000000	1.325261	1.031189
18	1	0	0.000000	-1.325261	1.031189

aug(d)-6-311G* basis set
E(RHF) = -1102.68205645
EUMP2 = -0.11040896026383D+04

6-31G* basis set
E(RHF) = -1102.57454119
EUMP2= -0.11038513147612D+04
CCSD(T)= -0.11039764510D+04

Dimer L, R = 7.0 A
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	16	0	0.000000	0.000000	4.689200
2	6	0	0.000000	1.233000	3.500000
3	6	0	0.000000	-1.233000	3.500000
4	6	0	0.000000	0.710208	2.222427
5	6	0	0.000000	-0.710208	2.222427
6	1	0	0.000000	2.272982	3.796782
7	1	0	0.000000	-2.272982	3.796782
8	1	0	0.000000	1.325261	1.330053
9	1	0	0.000000	-1.325261	1.330053
10	16	0	0.000000	0.000000	-4.689200
11	6	0	0.000000	-1.233000	-3.500000
12	6	0	0.000000	1.233000	-3.500000
13	6	0	0.000000	-0.710208	-2.222427
14	6	0	0.000000	0.710208	-2.222427
15	1	0	0.000000	-2.272982	-3.796782
16	1	0	0.000000	2.272982	-3.796782
17	1	0	0.000000	-1.325261	-1.330053
18	1	0	0.000000	1.325261	-1.330053

aug(d)-6-311G* basis set
E(RHF) = -1102.68187789
EUMP2 = -0.11040886248068D+04

6-31G* basis set
E(RHF) = -1102.57440039
EUMP2= -0.11038508216990D+04
CCSD(T)= -0.11039760679D+04

Dimer M, R = 6.6 A
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	0.000000	2.110800
2	6	0	0.000000	1.233000	3.300000
3	6	0	0.000000	-1.233000	3.300000
4	6	0	0.000000	0.710208	4.577573
5	6	0	0.000000	-0.710208	4.577573
6	1	0	0.000000	2.272982	3.003218
7	1	0	0.000000	-2.272982	3.003218
8	1	0	0.000000	1.325261	5.469947
9	1	0	0.000000	-1.325261	5.469947
10	16	0	0.000000	0.000000	-2.110800
11	6	0	0.000000	-1.233000	-3.300000
12	6	0	0.000000	1.233000	-3.300000
13	6	0	0.000000	-0.710208	-4.577573
14	6	0	0.000000	0.710208	-4.577573
15	1	0	0.000000	-2.272982	-3.003218
16	1	0	0.000000	2.272982	-3.003218
17	1	0	0.000000	-1.325261	-5.469947
18	1	0	0.000000	1.325261	-5.469947

aug(d)-6-311G* basis set

E(RHF) = -1102.68219645
EUMP2 = -0.11040886111011D+04

6-31G* basis set
E(RHF) = -1102.57463509
EUMP2= -0.11038507217240D+04
CCSD(T)= -0.11039758464D+04

Dimer N, R = 6.6 A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.225443	3.501210	0.000000
2	6	0	0.574163	1.986247	0.000000
3	6	0	1.259622	4.355065	0.000000
4	6	0	1.946706	2.133318	0.000000
5	6	0	2.341530	3.497756	0.000000
6	1	0	0.000000	1.069743	0.000000
7	1	0	1.263613	5.436558	0.000000
8	1	0	2.632951	1.294455	0.000000
9	1	0	3.369700	3.840523	0.000000
10	16	0	-0.587114	-2.026913	0.000000
11	6	0	-2.102078	-2.826519	0.000000
12	6	0	0.266741	-3.511978	0.000000
13	6	0	-1.955007	-4.199062	0.000000
14	6	0	-0.590568	-4.593886	0.000000
15	1	0	-3.018581	-2.252356	0.000000
16	1	0	1.348234	-3.515969	0.000000
17	1	0	-2.793869	-4.885307	0.000000
18	1	0	-0.247801	-5.622056	0.000000

aug(d)-6-311G* basis set
E(RHF) = -1102.68265048
EUMP2 = -0.11040889935269D+04

6-31G* basis set
E(RHF) = -1102.57513502
EUMP2= -0.11038512609792D+04
CCSD(T)= -0.11039764887D+04

Dimer O, R = 6.8 A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.282733	3.590508	0.000000
2	6	0	0.552385	2.094826	0.000000
3	6	0	1.181778	4.479154	0.000000
4	6	0	1.921077	2.274232	0.000000
5	6	0	2.283608	3.647604	0.000000
6	1	0	0.000000	1.165035	0.000000
7	1	0	1.160259	5.560440	0.000000

8	1	0	2.626918	1.451789	0.000000
9	1	0	3.303406	4.014527	0.000000
10	16	0	-1.171988	-4.437614	0.000000
11	6	0	0.323693	-3.602496	0.000000
12	6	0	-2.060635	-2.973103	0.000000
13	6	0	0.144288	-2.233804	0.000000
14	6	0	-1.229084	-1.871273	0.000000
15	1	0	1.253485	-4.154881	0.000000
16	1	0	-3.141921	-2.994622	0.000000
17	1	0	0.966730	-1.527963	0.000000
18	1	0	-1.596008	-0.851475	0.000000

aug(d)-6-311G* basis set
E(RHF) = -1102.68202535
EUMP2 = -0.11040887821385D+04

6-31G* basis set
(RHF) = -1102.57442561
EUMP2= -0.11038508097718D+04
CCSD(T)= -0.11039760277D+04

Dimer P, R = 7.0 A
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.189200	3.500000	0.000000
2	6	0	0.000000	2.267000	0.000000
3	6	0	0.000000	4.733000	0.000000
4	6	0	1.277573	2.789792	0.000000
5	6	0	1.277573	4.210208	0.000000
6	1	0	-0.296782	1.227018	0.000000
7	1	0	-0.296782	5.772982	0.000000
8	1	0	2.169947	2.174739	0.000000
9	1	0	2.169947	4.825261	0.000000
10	16	0	1.189200	-3.500000	0.000000
11	6	0	0.000000	-2.267000	0.000000
12	6	0	0.000000	-4.733000	0.000000
13	6	0	-1.277573	-2.789792	0.000000
14	6	0	-1.277573	-4.210208	0.000000
15	1	0	0.296782	-1.227018	0.000000
16	1	0	0.296782	-5.772982	0.000000
17	1	0	-2.169947	-2.174739	0.000000
18	1	0	-2.169947	-4.825261	0.000000

aug(d)-6-311G* basis set
E(RHF) = -1102.68210368
EUMP2 = -0.11040879337294D+04

6-31G* basis set
E(RHF) = -1102.57454767
EUMP2= -0.11038503304233D+04
CCSD(T)= -0.11039756128D+04

Dimer Q, R = 7.4 A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	3.700000	-1.190336
2	6	0	0.000000	4.933000	-0.001136
3	6	0	0.000000	2.467000	-0.001136
4	6	0	0.000000	4.410208	1.276436
5	6	0	0.000000	2.989792	1.276436
6	1	0	0.000000	5.972982	-0.297918
7	1	0	0.000000	1.427018	-0.297918
8	1	0	0.000000	5.025261	2.168811
9	1	0	0.000000	2.374739	2.168811
10	16	0	0.000000	-3.700000	-1.190336
11	6	0	0.000000	-2.467000	-0.001136
12	6	0	0.000000	-4.933000	-0.001136
13	6	0	0.000000	-2.989792	1.276436
14	6	0	0.000000	-4.410208	1.276436
15	1	0	0.000000	-1.427018	-0.297918
16	1	0	0.000000	-5.972982	-0.297918
17	1	0	0.000000	-2.374739	2.168811
18	1	0	0.000000	-5.025261	2.168811

aug(d)-6-311G* basis set
E(RHF) = -1102.68228293
EUMP2 = -0.11040876144547D+04

6-31G* basis set
E(RHF) = -1102.5747467
EUMP2= -0.11038501819854D+04
CCSD(T)= -0.11039754775D+04

Dimer B, MP2/6-311G** optimized geomerty

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.663083	2.153122	0.000000
2	6	0	-1.663083	0.963922	1.233000
3	6	0	-1.663083	0.963922	-1.233000
4	6	0	-1.663083	-0.313651	0.710208
5	6	0	-1.663083	-0.313651	-0.710208
6	1	0	-1.663083	1.260704	2.272982
7	1	0	-1.663083	1.260704	-2.272982
8	1	0	-1.663083	-1.206025	1.325261
9	1	0	-1.663083	-1.206025	-1.325261
10	16	0	1.663083	-2.153122	0.000000
11	6	0	1.663083	-0.963922	1.233000
12	6	0	1.663083	-0.963922	-1.233000
13	6	0	1.663083	0.313651	0.710208
14	6	0	1.663083	0.313651	-0.710208
15	1	0	1.663083	-1.260704	2.272982

16	1	0	1.663083	-1.260704	-2.272982
17	1	0	1.663083	1.206025	1.325261
18	1	0	1.663083	1.206025	-1.325261

MP2/6-31G
-0.11031886852825D+04
MP2/6-31G*
-0.11038540000000D+04
MP2/6-311G*
-0.11040204968726D+04
MP2/6-311G**
-0.11040808110613D+04
MP2/cc-pVDZ
-0.11039723761706D+04
MP2/cc-pVTZ
-0.11043922869805D+04
MP2/cc-pVQZ
-0.11045309938676D+04
MP2/cc-pVTZ(-f,d)
-0.11042249201522D+04
MP2/aug(d)-6-311G*
-0.11040979633632D+04
MP2/aug(d,p)-6-311G**
-0.11041594426411D+04
CCSD(T)/6-31G
-0.11032867705D+04
CCSD(T)/6-31G*
-0.11039770105D+04
CCSD(T)/6-311G*
-0.11041438769D+04
CCSD(T)/6-311G**
-0.11042076314D+04
CCSD(T)/cc-pVDZ
-0.11040955741D+04
CCSD(T)/cc-pVTZ(-f,d)
-0.11043518905D+04

Dimer I, MP2/6-311G** optimized geomerty
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.089079	2.022460	0.000000
2	6	0	-2.089079	0.833260	1.233000
3	6	0	-2.089079	0.833260	-1.233000
4	6	0	-2.089079	-0.444320	0.710210
5	6	0	-2.089079	-0.444320	-0.710210
6	1	0	-2.089079	1.130040	2.272980
7	1	0	-2.089079	1.130040	-2.272980
8	1	0	-2.089079	-1.336690	1.325260
9	1	0	-2.089079	-1.336690	-1.325260
10	16	0	1.165331	-1.582850	0.000000
11	6	0	1.310561	0.124020	0.000000
12	6	0	2.865831	-1.789690	0.000000
13	6	0	2.631731	0.524060	0.000000
14	6	0	3.527561	-0.578240	0.000000

15	1	0	0.424351	0.743910	0.000000
16	1	0	3.291411	-2.783940	0.000000
17	1	0	2.936341	1.564170	0.000000
18	1	0	4.607981	-0.492740	0.000000

MP2/6-31G
-0.11031912688643D+04
MP2/6-31G*
-0.11038560802770D+04
MP2/6-311G*
-0.11040220170695D+04
MP2/6-311G**
-0.11040820595974D+04
MP2/cc-pVDZ
-0.11039741805330D+04
MP2/cc-pVTZ
-0.11043930433985D+04
MP2/cc-pVQZ
-0.11045317001468D+04
MP2/cc-pVTZ(-f,d)
-0.11042256943816D+04
MP2/aug(d)-6-311G*
-0.11040970618828D+04
MP2/aug(d,p)-6-311G**
-0.11041586558853D+04
CCSD(T)/6-31G
-0.11032898741D+04
CCSD(T)/6-31G*
-0.11039800256D+04
CCSD(T)/6-311G*
-0.11041465438D+04
CCSD(T)/6-311G**
-0.11042100938D+04
CCSD(T)/cc-pVDZ
-0.11040986035D+04
CCSD(T)/cc-pVTZ(-f,d)
-0.11043540588D+04