

Supporting Information (SI)

For

Π -Stacking in Heterodimers of Propargylbenzene with (Fluoro)Phenylacetylenes

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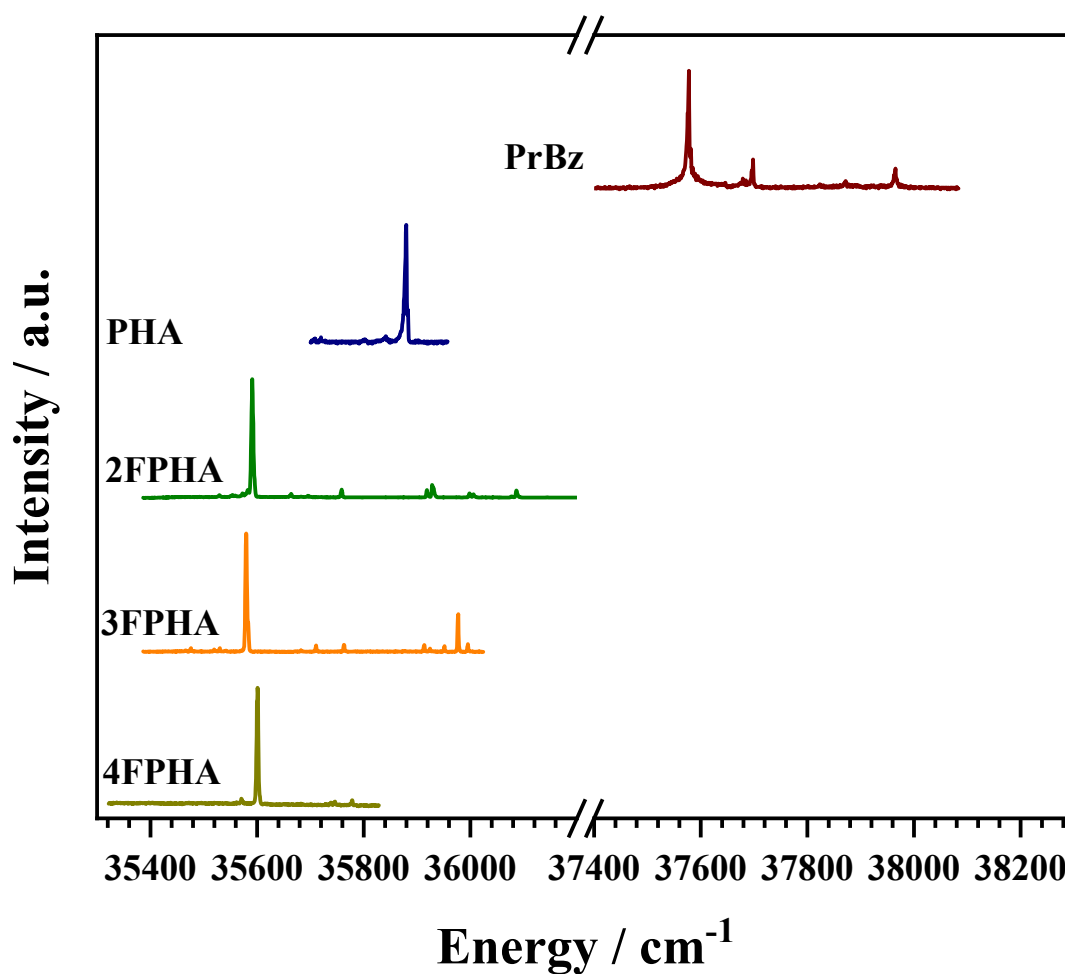


Figure S1. The electronic (1C-R2PI) spectra of monomers PrBz, PHA, 2FPHA, 3FPHA, and 4FPHA. The most intense band in each case is the band-origin (0_0^0) excitation of the $S_0 \rightarrow S_1$ transition.

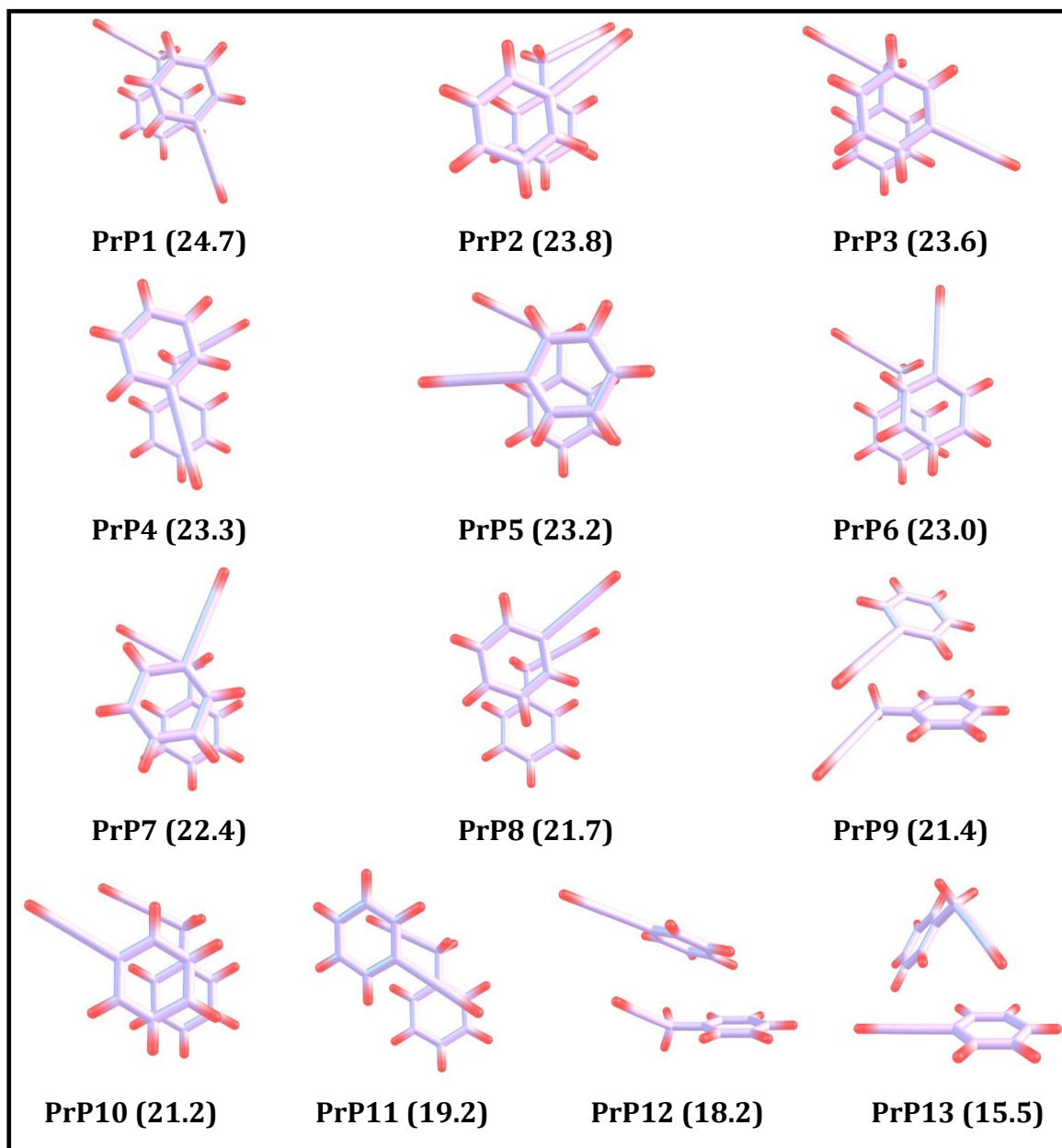


Figure S2. Structures of PrBz-PHA dimer optimized at M06-2X/aug-cc-pVDZ level. Structures are arranged in descending order with ZPE and BSSE corrected absolute value of stabilization energy (kJ mol^{-1}) (see Table S1).

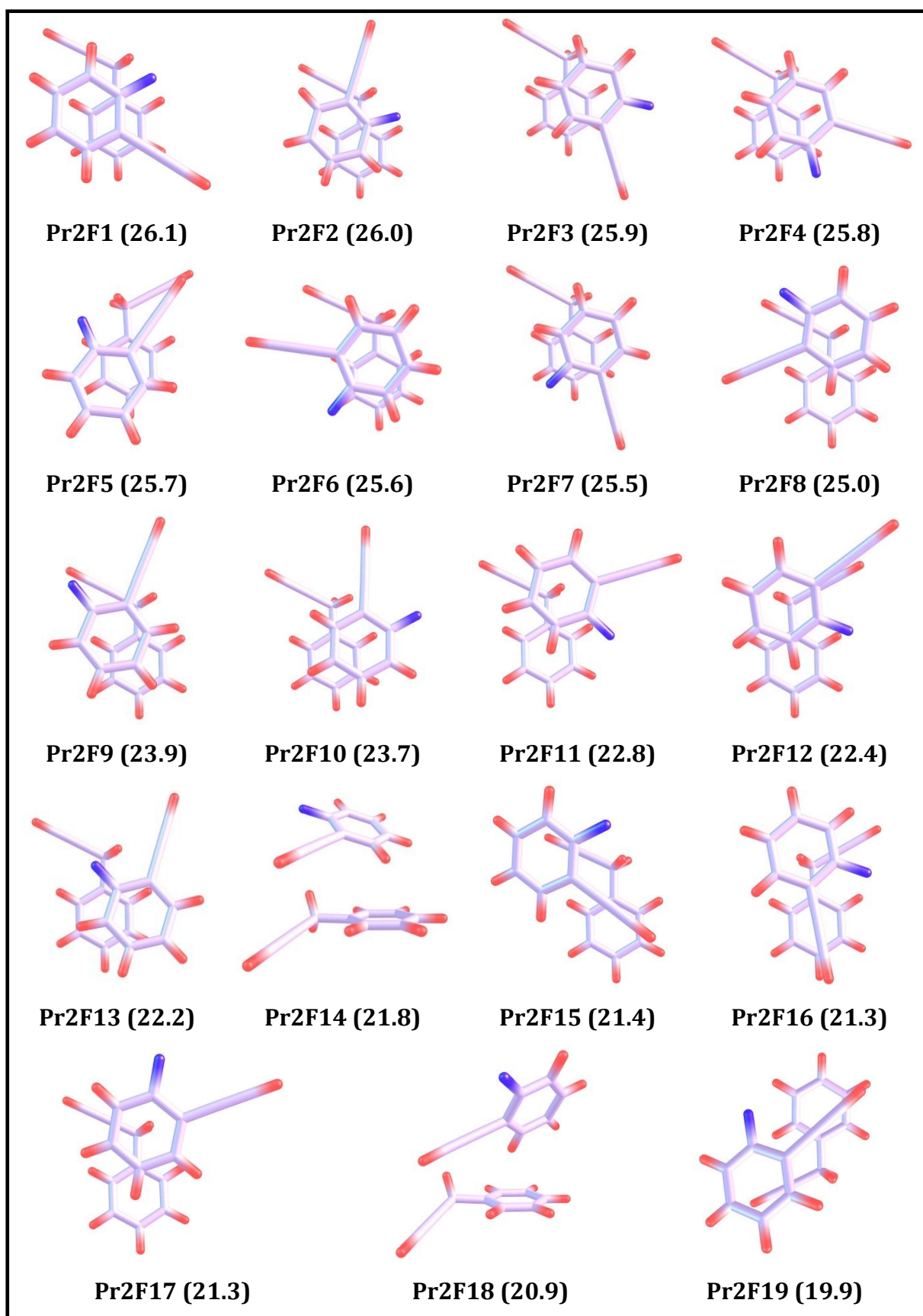


Figure S3. Structures of PrBz-2FPHA dimer optimized at M06-2X/aug-cc-pVDZ level. Structures are arranged in descending order with ZPE and BSSE corrected absolute value of stabilization energy (kJ mol^{-1}) (see Table S2).

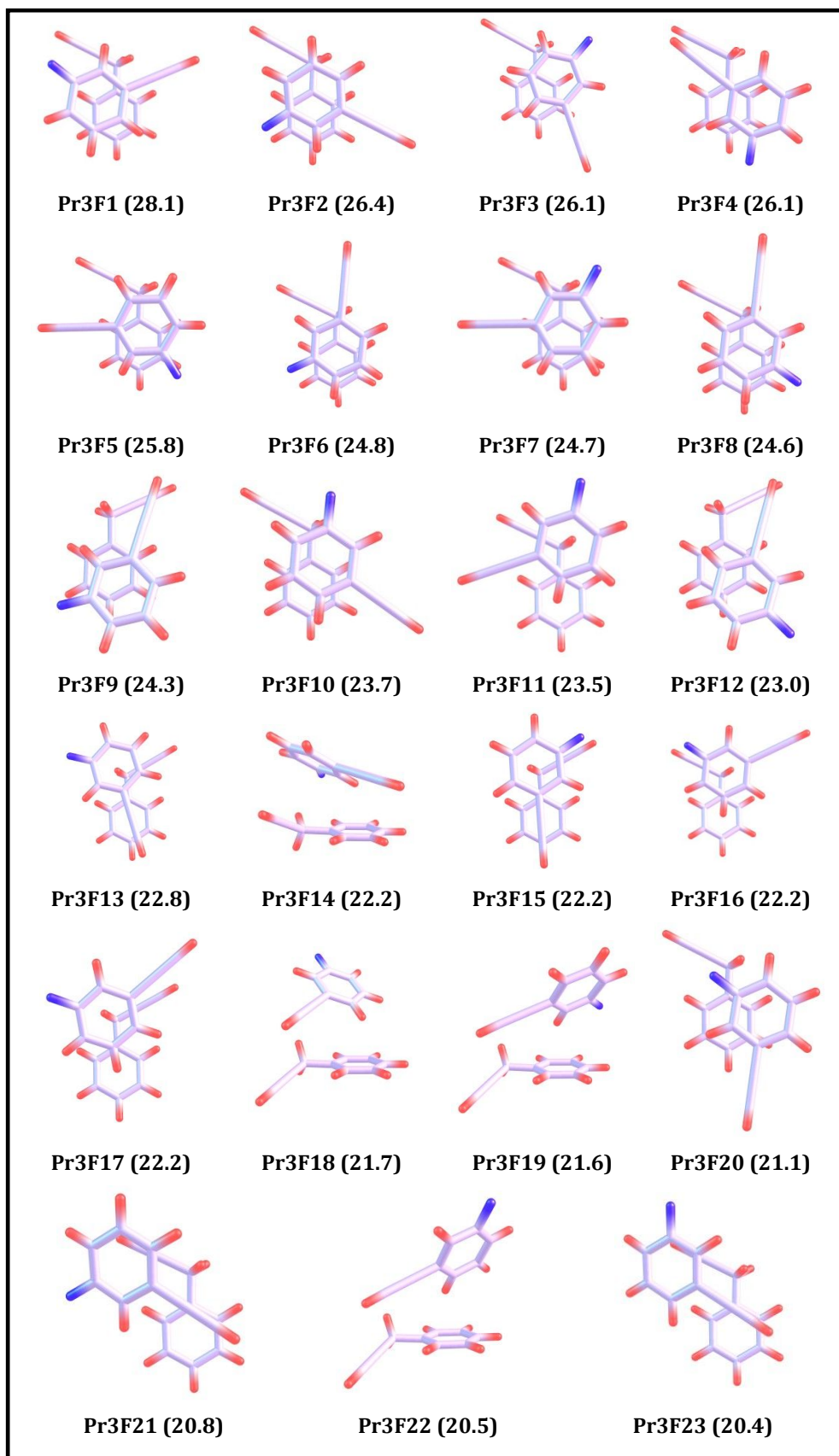


Figure S4. Structures of PrBz-3FPHA dimer optimized at M06-2X/aug-cc-pVDZ level. Structures are arranged in descending order with ZPE and BSSE corrected absolute value of stabilization energy (kJ mol^{-1}) (see Table S3).

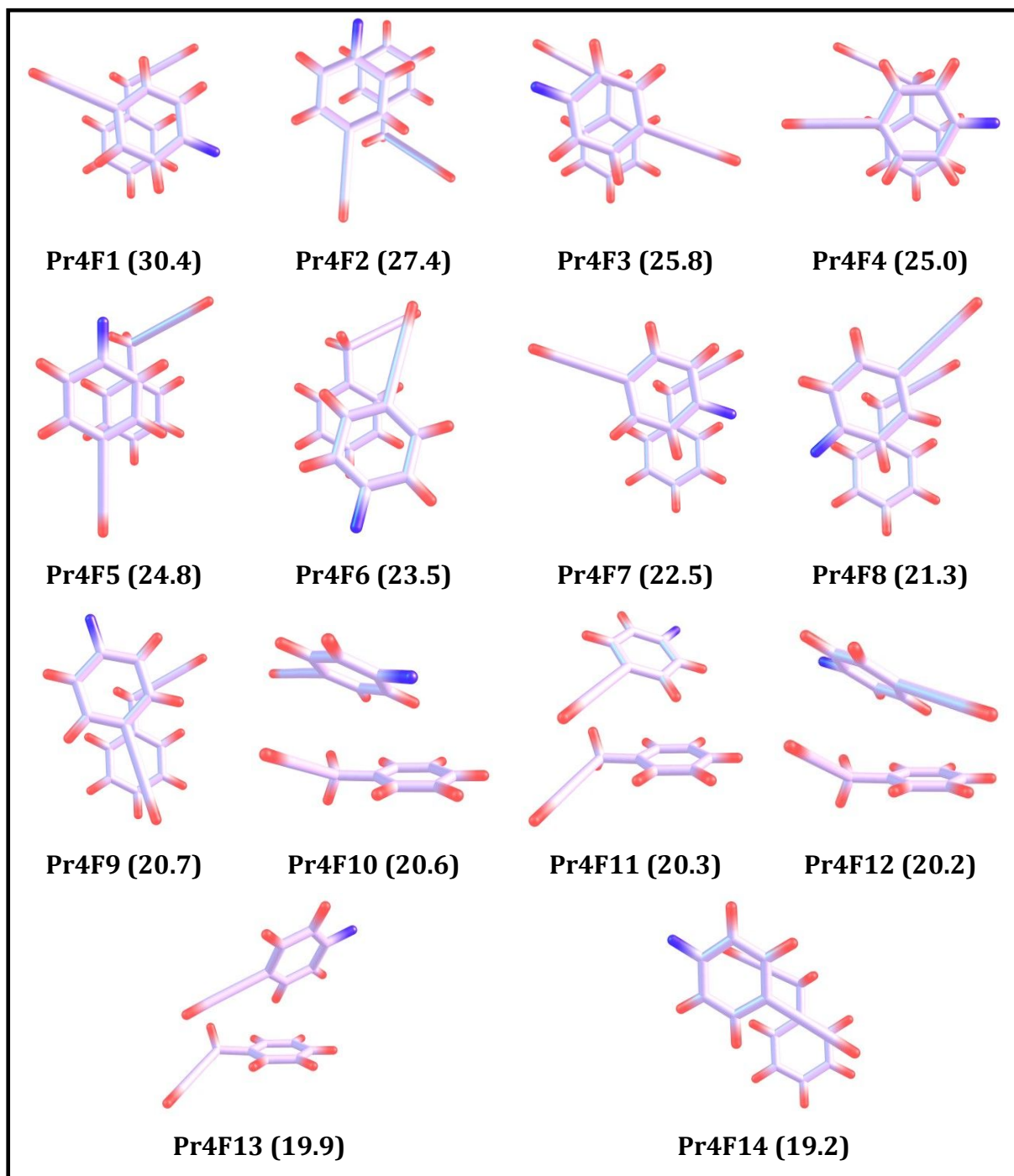


Figure S5. Structures of PrBz-4FPHA dimer optimized at M06-2X/aug-cc-pVDZ level. Structures are arranged in descending order with ZPE and BSSE corrected absolute value of stabilization energy (kJ mol^{-1}) (see Table S4).

Table S1. ZPE and BSSE corrected stabilization energies (kJ mol^{-1}), dipole moments (D) and SAPT0 interaction energy components (kJ mol^{-1}) for various structures of PrBz-PHA heterodimer.

Structure	M06-2X	MP2	μ	E_{Elec}	E_{Disp}	E_{Ind}	E_{CT}	E_{Exch}	E_{SAPT0}
PHA	-	-	0.71						
PrBz	-	-	0.53						
PrP1	-24.7	-33.6	0.5	-27.9	-65.6	-6.6	-0.5	64.0	-36.1
PrP2	-23.8	-32.1	1.1	-23.7	-65.7	-6.7	-0.6	62.2	-33.9
PrP3	-23.6	-32.9	0.3	-25.4	-64.9	-6.3	-0.4	61.9	-34.8
PrP4	-23.3	-28.9	0.7	-19.7	-60.7	-6.4	-0.7	55.9	-30.9
PrP5	-23.2	-32.6	0.9	-23.8	-66.9	-6.2	-0.5	63.0	-34.0
PrP6	-23.0	-31.6	0.9	-20.2	-62.2	-6.8	-0.6	59.0	-33.8
PrP7	-22.4	-31.0	0.7	-21.2	-64.6	-6.3	-0.6	60.2	-31.9
PrP8	-21.7	-28.2	1.0	-24.6	-56.4	-6.3	-0.7	56.0	-31.3
PrP9	-21.4	-27.1	1.0	-25.2	-53.2	-6.7	-0.8	53.9	-31.3
PrP10	-21.2	-29.5	1.1	-22.3	-63.6	-5.9	-0.4	61.2	-30.7
PrP11	-19.2	-25.8	0.3	-15.9	-56.8	-5.0	-0.5	52.0	-25.7
PrP12	-18.2	-25.3	1.3	-21.4	-54.6	-5.6	-0.5	53.4	-28.3
PrP13	-15.5	-20.0	0.6	-19.1	-41.3	-5.6	-0.8	41.2	-24.8

Table S2. ZPE and BSSE corrected stabilization energies (kJ mol⁻¹), dipole moments (D) and SAPT0 interaction energy components (kJ mol⁻¹) for various structures of PrBz-2FPHA heterodimer.

Structure	M06-2X	MP2	μ	E_{Elec}	E_{Disp}	E_{Ind}	E_{CT}	E_{Exch}	E_{SAPT0}
PrBz	-	-	0.53						
2FPHA	-	-	1.77						
Pr2F1	-26.1	-35.0	1.3	-27.9	-70.3	-6.4	-0.7	68.0	-36.7
Pr2F2	-26.0	-34.5	1.4	-26.1	-68.8	-6.8	-0.7	65.5	-36.3
Pr2F3	-25.9	-35.0	1.4	-29.3	-66.5	-6.5	-0.5	64.8	-37.5
Pr2F4	-25.8	-34.9	1.4	-30.3	-65.3	-6.4	-0.4	64.4	-37.7
Pr2F5	-25.7	-34.2	1.8	-29.1	-70.0	-6.5	-0.5	69.5	-36.2
Pr2F6	-25.6	-34.9	1.8	-29.9	-66.0	-6.2	-0.5	66.0	-36.2
Pr2F7	-25.5	-34.9	1.6	-29.4	-68.4	-6.4	-0.4	67.5	-36.7
Pr2F8	-25.0	-32.0	1.9	-28.8	-65.0	-6.8	-0.8	64.8	-35.7
Pr2F9	-23.9	-32.0	1.9	-25.2	-67.0	-6.4	-0.5	65.0	-33.6
Pr2F10	-23.7	-32.2	1.7	-25.2	-62.6	-6.8	-0.7	59.4	-35.2
Pr2F11	-22.8	-29.6	1.2	-27.0	-54.3	-6.1	-0.6	54.3	-33.1
Pr2F12	-22.4	-29.8	1.9	-26.7	-59.3	-6.6	-0.7	59.9	-32.7
Pr2F13	-22.2	-30.8	2.1	-24.1	-60.8	-6.7	-0.7	59.0	-32.6
Pr2F14	-21.8	-27.2	2	-26.1	-52.4	-6.8	-0.8	53.2	-32.0
Pr2F15	-21.4	-28.4	1.3	-19.0	-59.4	-5.1	-0.5	55.3	-28.3
Pr2F16	-21.3	-29.5	1.7	-19.1	-62.0	-6.4	-0.7	57.3	-30.2
Pr2F17	-21.3	-27.6	1.8	-24.3	-50.8	-5.4	-0.6	49.7	-30.8
Pr2F18	-20.9	-25.0	2.1	-27.8	-48.4	-6.8	-0.9	52.0	-31.1
Pr2F19	-19.9	-26.7	1.5	-17.4	-61.3	-5.3	-0.4	57.8	-26.2

Table S3. ZPE and BSSE corrected stabilization energies (kJ mol⁻¹), dipole moments (D) and SAPT0 interaction energy components (kJ mol⁻¹) for various structures of PrBz-3FPHA heterodimer.

Structure	M06-2X	MP2	μ	E_{Elec}	E_{Disp}	E_{Ind}	E_{CT}	E_{Exch}	E_{SAPT0}
PrBz	-	-	0.53						
3FPHA	-	-	1.40						
Pr3F1	-28.1	-36.8	1.7	-29.9	-71.0	-7.0	-0.7	69.1	-38.9
Pr3F2	-26.4	-36.0	1.4	-30.1	-69.6	-6.5	-0.5	68.5	-37.7
Pr3F3	-26.1	-35.1	1.4	-29.5	-66.0	-6.5	-0.5	64.3	-37.7
Pr3F4	-26.1	-34.7	1.3	-28.3	-68.6	-6.8	-0.6	66.8	-36.9
Pr3F5	-25.8	-35.7	1.1	-28.1	-70.6	-6.4	-0.6	68.1	-37.0
Pr3F6	-24.8	-33.9	1.6	-25.6	-66.9	-6.4	-0.6	63.9	-35.1
Pr3F7	-24.7	-34.2	1.5	-25.1	-67.9	-6.0	-0.5	63.8	-35.4
Pr3F8	-24.6	-34.0	1.0	-25.4	-66.0	-6.6	-0.6	62.6	-35.5
Pr3F9	-24.3	-32.7	1.0	-28.5	-64.5	-5.9	-0.5	64.5	-34.5
Pr3F10	-23.7	-33.2	1.4	-25.1	-65.6	-6.4	-0.5	62.2	-34.9
Pr3F11	-23.5	-30.9	1.6	-24.9	-62.1	-6.0	-0.8	59.7	-33.4
Pr3F12	-23.0	-31.0	1.7	-25.9	-61.8	-5.7	-0.4	60.9	-32.4
Pr3F13	-22.8	-29.9	1.1	-20.2	-60.3	-6.2	-0.7	55.5	-31.2
Pr3F14	-22.2	-29.7	0.8	-25.8	-62.1	-6.5	-0.6	61.3	-33.0
Pr3F15	-22.2	-29.1	1.6	-25.1	-56.2	-6.2	-0.6	55.7	-31.8
Pr3F16	-22.2	-28.5	1.6	-22.3	-63.3	-6.5	-0.7	61.3	-30.9
Pr3F17	-22.2	-28.5	1.3	-25.1	-56.2	-6.2	-0.6	55.7	-31.8
Pr3F18	-21.7	-27.2	1.5	-25.4	-52.1	-6.5	-0.8	52.6	-31.4
Pr3F19	-21.6	-26.3	0.9	-28.5	-50.9	-6.8	-0.8	54.7	-31.5
Pr3F20	-21.1	-30.3	1.8	-21.6	-62.1	-5.9	-0.6	58.5	-31.1
Pr3F21	-20.8	-27.6	1.7	-18.1	-56.8	-4.8	-0.4	52.4	-27.3
Pr3F22	-20.5	-24.8	1.8	-27.0	-48.0	-6.5	-0.8	51.0	-30.5
Pr3F23	-20.4	-27.2	1.4	-17.8	-57.0	-4.9	-0.4	52.9	-26.7

Table S4. ZPE and BSSE corrected stabilization energies (kJ mol⁻¹), dipole moments (D) and SAPT0 interaction energy components (kJ mol⁻¹) for various structures of PrBz-4FPHA heterodimer.

Structure	M06-2X	MP2	μ	E_{Elec}	E_{Disp}	E_{Ind}	E_{CT}	E_{Exch}	E_{SAPT0}
PrBz	-	-	0.53						
4FPHA	-	-	0.85						
Pr4F1	-30.4	-37.4	1.2	-29.3	-69.4	-6.9	-0.7	65.8	-39.8
Pr4F2	-27.4	-34.8	0.8	-28.7	-65.7	-6.96	-0.7	64.3	-37.1
Pr4F3	-25.8	-34.7	1.1	-28.2	-65.6	-6.89	-0.7	63.8	-36.9
Pr4F4	-25.0	-34.7	0.7	-26.7	-68.0	-6.34	-0.5	64.7	-36.4
Pr4F5	-24.8	-33.4	1.1	-25.5	-64.3	-6.09	-0.6	61.2	-34.7
Pr4F6	-23.5	-31.2	0.7	-26.2	-61.9	-5.65	-0.5	61.1	-32.6
Pr4F7	-22.5	-29.6	1.0	-26.2	-58.4	-6.43	-0.7	58.7	-32.4
Pr4F8	-21.3	-29.3	0.4	-26.0	-55.1	-5.9	-0.6	54.6	-32.3
Pr4F9	-20.7	-29.3	1.1	-26.5	-52.6	-6.87	-0.8	53.4	-32.6
Pr4F10	-20.6	-28	1.0	-18.9	-59.7	-5.92	-0.7	54.6	-29.9
Pr4F11	-20.3	-27.6	0.7	-23.8	-59.3	-6.26	-0.6	57.1	-32.3
Pr4F12	-20.2	-28.8	1.1	-28.2	-48.5	-6.95	-0.9	52.1	-31.6
Pr4F13	-19.9	-25.3	0.9	-18.9	-57.8	-5.04	-0.5	53.8	-27.9
Pr4F14	-19.2	-27.6	1.4	-22.5	-55.1	-5.59	-0.5	53.2	-30.1

Optimized coordinates (in angstrom) of various hetero-dimers of PrBz with PHA, 2FPHA, 3FPHA and 4FPHA calculated at M06-2X/aug-cc-pVDZ level of theory.

PrBz-PHA Hetero-Dimer

PrP1

C	1.78354000000	0.44109200000	0.50445200000
C	0.88282900000	1.48450700000	0.70191100000
C	-0.23270900000	1.30364300000	1.52114100000
C	-0.44489500000	0.07355600000	2.14492500000
C	0.45280400000	-0.97261100000	1.95609200000
C	1.57202000000	-0.79551400000	1.13085600000
C	2.48072100000	-1.88559100000	0.90537400000
C	3.23693400000	-2.80969100000	0.70394000000
H	2.65316100000	0.57105700000	-0.13695800000
H	1.05368700000	2.44338000000	0.21434000000
H	-0.94640300000	2.11370900000	1.66605100000
H	-1.32810600000	-0.07481000000	2.76385000000
H	0.28458100000	-1.94041300000	2.42385700000
H	3.91341000000	-3.62111800000	0.53788500000
C	-0.22084500000	-2.39240500000	-1.20481900000
C	-0.87207400000	-1.16277300000	-1.27852200000
C	-2.03621300000	-0.92913200000	-0.54336300000
C	-2.54966400000	-1.94930400000	0.25963600000
C	-1.90147300000	-3.18199000000	0.33192000000
C	-0.73243100000	-3.40580300000	-0.39518900000
C	-2.71728700000	0.42425200000	-0.65265700000
C	-3.49195500000	0.80774000000	0.53053700000
C	-4.13427900000	1.11829200000	1.50709400000
H	0.70268800000	-2.55164700000	-1.75937000000
H	-0.45526600000	-0.36537800000	-1.89447000000
H	-3.44913800000	-1.76882300000	0.84701700000
H	-2.30752800000	-3.96857800000	0.96668300000
H	-0.21484400000	-4.36101500000	-0.32315700000
H	-3.38692900000	0.43057700000	-1.52455000000
H	-1.95313700000	1.19092400000	-0.83377600000
H	-4.70907200000	1.40083600000	2.36367600000

PrP2

C	-5.256508000000	2.563947000000	-0.644733000000
C	-5.947926000000	1.647358000000	-1.431541000000
C	-5.902917000000	0.286555000000	-1.125447000000
C	-5.161620000000	-0.155887000000	-0.029548000000
C	-4.463163000000	0.753208000000	0.758548000000
C	-4.506715000000	2.120850000000	0.455282000000
C	-3.761501000000	3.061162000000	1.244894000000
C	-3.096281000000	3.854652000000	1.872387000000
H	-5.291379000000	3.628265000000	-0.871801000000
H	-6.528176000000	1.996660000000	-2.284172000000
H	-6.444840000000	-0.428592000000	-1.742411000000
H	-5.116322000000	-1.217961000000	0.206159000000
H	-3.865698000000	0.414388000000	1.602244000000
H	-2.501458000000	4.553029000000	2.421865000000
C	-2.302832000000	-0.286363000000	-1.859213000000
C	-2.259127000000	1.095359000000	-2.019231000000
C	-1.583738000000	1.900348000000	-1.095368000000
C	-0.960514000000	1.300319000000	-0.001952000000
C	-1.006181000000	-0.085813000000	0.161954000000
C	-1.672634000000	-0.883202000000	-0.765713000000
C	-1.591264000000	3.404104000000	-1.307524000000
C	-0.647053000000	4.151543000000	-0.475995000000
C	0.144178000000	4.760994000000	0.205656000000
H	-2.834466000000	-0.898641000000	-2.586295000000
H	-2.760238000000	1.558159000000	-2.870221000000
H	-0.438727000000	1.921720000000	0.723827000000
H	-0.511757000000	-0.542943000000	1.018137000000
H	-1.702896000000	-1.964429000000	-0.638488000000
H	-2.604307000000	3.783901000000	-1.110153000000
H	-1.372276000000	3.617629000000	-2.361831000000
H	0.845849000000	5.309308000000	0.797740000000

PrP3

C	0.360882000000	1.385472000000	1.106992000000
C	-0.620687000000	1.169150000000	2.070734000000
C	-0.783888000000	-0.096833000000	2.632963000000
C	0.046325000000	-1.146739000000	2.237452000000
C	1.028705000000	-0.939685000000	1.275112000000
C	1.186082000000	0.328066000000	0.697199000000
C	2.162559000000	0.532332000000	-0.336620000000
C	2.964465000000	0.697233000000	-1.228960000000
H	0.492389000000	2.367849000000	0.656550000000
H	-1.272459000000	1.986220000000	2.375379000000
H	-1.568138000000	-0.266528000000	3.368168000000
H	-0.084175000000	-2.137912000000	2.668470000000
H	1.664236000000	-1.758061000000	0.944114000000
H	3.688062000000	0.848240000000	-2.001626000000
C	-0.145065000000	-1.828163000000	-1.849665000000
C	-0.952819000000	-0.736686000000	-1.540552000000
C	-2.027378000000	-0.870717000000	-0.656482000000
C	-2.283786000000	-2.118006000000	-0.085706000000
C	-1.477746000000	-3.214081000000	-0.395261000000
C	-0.406581000000	-3.073132000000	-1.276269000000
C	-2.893747000000	0.345782000000	-0.376692000000
C	-3.749181000000	0.235586000000	0.806249000000
C	-4.462533000000	0.139212000000	1.778036000000
H	0.699149000000	-1.700163000000	-2.525506000000
H	-0.729942000000	0.238495000000	-1.975663000000
H	-3.110442000000	-2.226786000000	0.614882000000
H	-1.686769000000	-4.182318000000	0.058013000000
H	0.224676000000	-3.928377000000	-1.512979000000

H	-3.532903000000	0.541572000000	-1.249255000000
H	-2.244168000000	1.222335000000	-0.258525000000
H	-5.100977000000	0.063723000000	2.632722000000

PrP4

C	-4.177280000000	3.838319000000	0.665950000000
C	-4.284462000000	5.096133000000	0.077411000000
C	-4.972419000000	5.252519000000	-1.125758000000
C	-5.553132000000	4.142165000000	-1.744265000000
C	-5.452147000000	2.882536000000	-1.160738000000
C	-4.764503000000	2.722983000000	0.052594000000
C	-4.652351000000	1.423095000000	0.652609000000
C	-4.552039000000	0.325510000000	1.152124000000
H	-3.626095000000	3.705971000000	1.594754000000
H	-3.812659000000	5.954037000000	0.552634000000
H	-5.050997000000	6.235983000000	-1.585892000000
H	-6.087301000000	4.259686000000	-2.685781000000
H	-5.898418000000	2.010801000000	-1.635543000000
H	-4.452817000000	-0.645372000000	1.588631000000
C	-2.478437000000	-0.404888000000	-1.787241000000
C	-2.458961000000	0.953101000000	-2.086906000000
C	-1.760849000000	1.854976000000	-1.275062000000
C	-1.090549000000	1.374106000000	-0.152061000000
C	-1.107866000000	0.010429000000	0.150156000000
C	-1.796394000000	-0.882544000000	-0.665882000000
C	-1.757038000000	3.321354000000	-1.672748000000
C	-1.077984000000	4.214798000000	-0.733888000000
C	-0.504727000000	4.941413000000	0.044529000000
H	-3.026579000000	-1.094107000000	-2.428105000000
H	-2.994647000000	1.325117000000	-2.961444000000
H	-0.551386000000	2.069185000000	0.489229000000
H	-0.577737000000	-0.352078000000	1.029910000000
H	-1.807841000000	-1.945810000000	-0.430177000000
H	-2.794021000000	3.662574000000	-1.796652000000
H	-1.275650000000	3.420613000000	-2.655487000000
H	0.002483000000	5.594945000000	0.722224000000

PrP5

C	-0.515228000000	0.592581000000	2.279492000000
C	0.413872000000	1.253153000000	1.479131000000
C	1.412089000000	0.533942000000	0.820786000000
C	1.484692000000	-0.852214000000	0.969461000000
C	0.562452000000	-1.519259000000	1.767886000000
C	-0.447000000000	-0.800023000000	2.425022000000
C	-1.415418000000	-1.492932000000	3.228775000000
C	-2.233878000000	-2.084306000000	3.896974000000
H	-1.306630000000	1.141633000000	2.784934000000
H	0.358285000000	2.335425000000	1.370025000000
H	2.134714000000	1.053667000000	0.193439000000
H	2.256666000000	-1.418069000000	0.450686000000
H	0.600920000000	-2.601145000000	1.875845000000
H	-2.950625000000	-2.604169000000	4.496402000000
C	-0.217466000000	-2.262306000000	-1.803982000000
C	-0.851776000000	-1.044150000000	-1.573220000000
C	-1.918424000000	-0.954194000000	-0.673913000000
C	-2.342933000000	-2.104468000000	-0.008118000000
C	-1.706365000000	-3.325038000000	-0.234326000000
C	-0.642913000000	-3.408952000000	-1.131691000000
C	-2.586280000000	0.396338000000	-0.472987000000
C	-3.466542000000	0.471616000000	0.693879000000
C	-4.185591000000	0.510182000000	1.664950000000
H	0.614631000000	-2.316284000000	-2.504790000000

H	-0.507288000000	-0.147080000000	-2.089238000000
H	-3.157144000000	-2.038819000000	0.711554000000
H	-2.040863000000	-4.212812000000	0.300717000000
H	-0.146502000000	-4.362367000000	-1.306905000000
H	-3.167619000000	0.649857000000	-1.370555000000
H	-1.806700000000	1.163046000000	-0.373552000000
H	-4.818474000000	0.549711000000	2.526018000000

PrP6

C	1.397770000000	1.057101000000	0.874125000000
C	2.051794000000	-0.170303000000	0.839556000000
C	1.481572000000	-1.286956000000	1.453609000000
C	0.255126000000	-1.172706000000	2.106581000000
C	-0.403937000000	0.052771000000	2.150497000000
C	0.163564000000	1.175918000000	1.531712000000
C	-0.525539000000	2.437233000000	1.558091000000
C	-1.125055000000	3.489309000000	1.562137000000
H	1.833151000000	1.933102000000	0.397006000000
H	3.008958000000	-0.257392000000	0.327584000000
H	1.988778000000	-2.249598000000	1.413130000000
H	-0.199733000000	-2.045849000000	2.570969000000
H	-1.370876000000	0.148706000000	2.640777000000
H	-1.652108000000	4.419617000000	1.580885000000
C	-0.123014000000	-2.141386000000	-1.457740000000
C	-0.806589000000	-0.940566000000	-1.282349000000
C	-1.992504000000	-0.897921000000	-0.544872000000
C	-2.485467000000	-2.076991000000	0.016524000000
C	-1.802400000000	-3.280847000000	-0.158261000000
C	-0.619761000000	-3.317699000000	-0.895770000000
C	-2.719136000000	0.427866000000	-0.398986000000
C	-3.585877000000	0.519250000000	0.777877000000
C	-4.303605000000	0.586428000000	1.748848000000
H	0.807096000000	-2.156176000000	-2.024374000000
H	-0.403368000000	-0.019980000000	-1.705246000000
H	-3.401033000000	-2.047707000000	0.605788000000
H	-2.196311000000	-4.194229000000	0.285835000000
H	-0.085082000000	-4.257165000000	-1.028068000000
H	-3.330289000000	0.606060000000	-1.295365000000
H	-1.984070000000	1.241226000000	-0.351743000000
H	-4.939779000000	0.660914000000	2.605133000000

PrP7

C	2.597807000000	-1.944190000000	0.804544000000
C	2.768524000000	-2.136025000000	2.171929000000
C	1.838647000000	-1.619389000000	3.075299000000
C	0.735330000000	-0.905207000000	2.609104000000
C	0.553117000000	-0.716981000000	1.242296000000
C	1.482329000000	-1.238400000000	0.330295000000
C	1.297931000000	-1.042158000000	-1.081335000000
C	1.146580000000	-0.858334000000	-2.268593000000
H	3.323158000000	-2.329869000000	0.091486000000
H	3.635227000000	-2.686235000000	2.534998000000
H	0.019620000000	-0.483607000000	3.312679000000
H	-0.304678000000	-0.160317000000	0.868848000000
H	1.014757000000	-0.709551000000	-3.319242000000
C	1.285299000000	2.683751000000	3.251258000000
C	1.564160000000	2.579887000000	1.892457000000
C	2.701032000000	1.895535000000	1.444481000000
C	3.553926000000	1.317845000000	2.381980000000
C	3.277993000000	1.424310000000	3.747426000000
C	2.146165000000	2.104488000000	4.187199000000
C	2.955239000000	1.827795000000	-0.051683000000

C	4.091873000000	0.997628000000	-0.451002000000
C	5.039416000000	0.319934000000	-0.774587000000
H	0.396944000000	3.219449000000	3.583500000000
H	0.889300000000	3.031751000000	1.164136000000
H	4.433719000000	0.773998000000	2.042307000000
H	3.953085000000	0.966261000000	4.469342000000
H	1.932464000000	2.186487000000	5.251895000000
H	3.118907000000	2.846276000000	-0.430649000000
H	2.055851000000	1.447699000000	-0.554605000000
H	5.872833000000	-0.277777000000	-1.076788000000
H	1.981996000000	-1.760218000000	4.145433000000

PrP8

C	-4.818837000000	5.127932000000	-0.551248000000
C	-5.370104000000	4.186843000000	-1.417983000000
C	-5.212176000000	2.822697000000	-1.166795000000
C	-4.495392000000	2.399270000000	-0.046700000000
C	-3.939977000000	3.333680000000	0.821974000000
C	-4.102119000000	4.705918000000	0.578031000000
C	-3.542667000000	5.673178000000	1.481122000000
C	-3.088335000000	6.491268000000	2.249102000000
H	-4.937023000000	6.193239000000	-0.738897000000
H	-5.925844000000	4.520787000000	-2.292809000000
H	-5.638278000000	2.088222000000	-1.848559000000
H	-4.343981000000	1.335776000000	0.135037000000
H	-3.364101000000	3.012400000000	1.687629000000
H	-2.687781000000	7.215743000000	2.926082000000
C	-2.513725000000	-0.324835000000	-2.141731000000
C	-2.314762000000	1.036373000000	-2.352826000000
C	-1.672319000000	1.823305000000	-1.390829000000
C	-1.214420000000	1.220253000000	-0.220731000000
C	-1.412272000000	-0.145863000000	-0.005786000000
C	-2.065681000000	-0.921526000000	-0.960677000000
C	-1.547279000000	3.313953000000	-1.651021000000
C	-0.908822000000	4.076205000000	-0.578224000000
C	-0.396676000000	4.701392000000	0.320662000000
H	-3.020022000000	-0.923472000000	-2.897881000000
H	-2.678816000000	1.502852000000	-3.269268000000
H	-0.714066000000	1.826584000000	0.532697000000
H	-1.053093000000	-0.604124000000	0.914750000000
H	-2.222052000000	-1.985698000000	-0.790883000000
H	-2.556223000000	3.722456000000	-1.811943000000
H	-0.989537000000	3.473521000000	-2.583687000000
H	0.039109000000	5.274704000000	1.111030000000

PrP9

C	0.940270000000	-1.097367000000	1.803102000000
C	2.254687000000	-1.201572000000	1.356929000000
C	3.169325000000	-0.180612000000	1.615160000000
C	2.765583000000	0.953379000000	2.322408000000
C	1.453725000000	1.066004000000	2.772301000000
C	0.532124000000	0.038666000000	2.516516000000
C	-0.826898000000	0.159916000000	2.968551000000
C	-1.978613000000	0.280147000000	3.322377000000
H	0.218506000000	-1.883811000000	1.588568000000
H	2.561868000000	-2.084604000000	0.798415000000
H	4.197003000000	-0.266108000000	1.264964000000
H	3.476685000000	1.752773000000	2.525184000000
H	1.129820000000	1.945554000000	3.325666000000
H	-3.000591000000	0.387928000000	3.618121000000
C	-0.028757000000	-2.083779000000	-1.416069000000
C	-0.489564000000	-0.786916000000	-1.201688000000

C	-1.605349000000	-0.549534000000	-0.393129000000
C	-2.257620000000	-1.633779000000	0.195553000000
C	-1.796560000000	-2.934187000000	-0.015211000000
C	-0.680703000000	-3.164136000000	-0.819733000000
C	-2.035760000000	0.886169000000	-0.147628000000
C	-3.401422000000	1.037726000000	0.356865000000
C	-4.535113000000	1.154452000000	0.761028000000
H	0.842268000000	-2.251419000000	-2.048069000000
H	0.029921000000	0.054771000000	-1.660766000000
H	-3.127948000000	-1.456074000000	0.824797000000
H	-2.314333000000	-3.771437000000	0.450365000000
H	-0.324831000000	-4.179665000000	-0.986450000000
H	-1.943727000000	1.454348000000	-1.082054000000
H	-1.344657000000	1.343642000000	0.575447000000
H	-5.539854000000	1.272427000000	1.107680000000

PrP10

C	-2.582305000000	1.416225000000	4.193278000000
C	-1.865327000000	2.432423000000	3.569632000000
C	-0.483240000000	2.318471000000	3.376882000000
C	0.169549000000	1.170492000000	3.820101000000
C	-0.547916000000	0.151705000000	4.451235000000
C	-1.922145000000	0.268422000000	4.638988000000
C	0.243522000000	3.462296000000	2.689005000000
C	1.660640000000	3.216992000000	2.419762000000
C	2.825899000000	2.987916000000	2.194409000000
H	-3.657399000000	1.518740000000	4.335214000000
H	-2.383866000000	3.327134000000	3.221860000000
H	1.241468000000	1.066417000000	3.659300000000
H	-0.025598000000	-0.742574000000	4.788929000000
H	-2.480012000000	-0.528042000000	5.129257000000
H	0.149703000000	4.368481000000	3.303173000000
H	-0.260334000000	3.677850000000	1.736483000000
H	3.852479000000	2.779430000000	1.979868000000
C	0.490142000000	-1.010055000000	1.111526000000
C	-0.894272000000	-0.952339000000	1.247807000000
C	-1.596350000000	0.166592000000	0.803025000000
C	-0.909327000000	1.228168000000	0.211421000000
C	0.474447000000	1.181701000000	0.076023000000
C	1.184361000000	0.059982000000	0.530825000000
C	2.614285000000	0.005182000000	0.400432000000
C	3.818556000000	-0.053582000000	0.287343000000
H	1.047087000000	-1.877523000000	1.460698000000
H	-1.426111000000	-1.779100000000	1.715481000000
H	-2.677078000000	0.215578000000	0.924145000000
H	-1.457557000000	2.100970000000	-0.141346000000
H	1.021941000000	2.010295000000	-0.368778000000
H	4.880891000000	-0.111384000000	0.178745000000

PrP11

C	-3.081205000000	0.909879000000	3.379923000000
C	-4.446058000000	0.694551000000	3.542255000000
C	-5.099248000000	-0.270912000000	2.775970000000
C	-4.383474000000	-1.020820000000	1.841741000000
C	-3.018732000000	-0.810032000000	1.672620000000
C	-2.357454000000	0.157717000000	2.443130000000
C	-0.948061000000	0.375274000000	2.269627000000
C	0.235531000000	0.565299000000	2.100523000000
H	-2.562909000000	1.658839000000	3.976097000000
H	-5.002604000000	1.283493000000	4.269463000000
H	-6.167387000000	-0.438934000000	2.906670000000
H	-4.891706000000	-1.774737000000	1.242521000000

H	-2.449521000000	-1.385479000000	0.945092000000
H	1.280136000000	0.726855000000	1.939040000000
C	0.738027000000	1.571996000000	-1.550752000000
C	-0.113753000000	2.394253000000	-0.819780000000
C	-1.446206000000	2.028889000000	-0.601523000000
C	-1.918150000000	0.835110000000	-1.143485000000
C	-1.064123000000	0.005585000000	-1.873651000000
C	0.265287000000	0.366999000000	-2.075783000000
C	-2.307751000000	2.929210000000	0.265943000000
C	-3.725572000000	2.570716000000	0.308156000000
C	-4.893858000000	2.261690000000	0.335459000000
H	1.773428000000	1.869392000000	-1.712758000000
H	0.261749000000	3.328666000000	-0.400422000000
H	-2.957431000000	0.551344000000	-0.984807000000
H	-1.443212000000	-0.927574000000	-2.288807000000
H	0.930122000000	-0.280391000000	-2.645583000000
H	-2.213221000000	3.966179000000	-0.082195000000
H	-1.908942000000	2.902376000000	1.291228000000
H	-5.928308000000	1.994561000000	0.373345000000

PrP12

C	-3.123094000000	1.762625000000	3.934110000000
C	-2.142972000000	2.581805000000	3.375170000000
C	-0.787889000000	2.328810000000	3.601943000000
C	-0.425613000000	1.250130000000	4.410026000000
C	-1.403267000000	0.431681000000	4.974552000000
C	-2.754817000000	0.681283000000	4.735091000000
C	0.254256000000	3.230150000000	2.963691000000
C	1.533315000000	2.568684000000	2.695208000000
C	2.580649000000	2.013312000000	2.459519000000
H	-4.175303000000	1.965740000000	3.739949000000
H	-2.435289000000	3.418968000000	2.740088000000
H	0.629835000000	1.033464000000	4.569353000000
H	-1.107859000000	-0.411560000000	5.597535000000
H	-3.517346000000	0.036106000000	5.168489000000
H	0.430826000000	4.102553000000	3.609169000000
H	-0.141489000000	3.614811000000	2.014644000000
H	3.501416000000	1.523536000000	2.220527000000
C	1.365928000000	-0.876407000000	0.845984000000
C	0.185240000000	-0.923406000000	1.580845000000
C	-0.825317000000	0.008294000000	1.346433000000
C	-0.652757000000	0.987684000000	0.367125000000
C	0.525618000000	1.043329000000	-0.371024000000
C	1.546346000000	0.112656000000	-0.131339000000
C	2.782817000000	0.187668000000	-0.859442000000
C	3.834797000000	0.258153000000	-1.455202000000
H	2.162426000000	-1.595767000000	1.027220000000
H	0.054991000000	-1.684854000000	2.348288000000
H	-1.738357000000	-0.015383000000	1.940867000000
H	-1.441440000000	1.716847000000	0.184286000000
H	0.673461000000	1.810216000000	-1.128894000000
H	4.757755000000	0.316508000000	-1.992335000000

PrP13

C	-3.771525000000	-0.445004000000	3.143736000000
C	-3.843870000000	0.907742000000	3.462950000000
C	-5.083105000000	1.522725000000	3.641733000000
C	-6.256934000000	0.779649000000	3.499272000000
C	-6.193298000000	-0.573774000000	3.179040000000
C	-4.947906000000	-1.194426000000	2.999776000000
C	-4.881205000000	-2.589512000000	2.660899000000
C	-4.828773000000	-3.762051000000	2.363123000000

H	-2.808379000000	-0.927140000000	2.987069000000
H	-2.927588000000	1.486557000000	3.563882000000
H	-5.135626000000	2.581538000000	3.890458000000
H	-7.225838000000	1.256183000000	3.640276000000
H	-7.102066000000	-1.161459000000	3.064879000000
H	-4.786008000000	-4.798874000000	2.103723000000
C	0.346017000000	-2.078053000000	-0.395839000000
C	-0.464942000000	-1.122448000000	-1.006771000000
C	-1.824444000000	-1.038846000000	-0.695198000000
C	-2.362496000000	-1.927375000000	0.238198000000
C	-1.553255000000	-2.882831000000	0.851834000000
C	-0.196546000000	-2.961566000000	0.537330000000
C	-2.694837000000	-0.010381000000	-1.399921000000
C	-3.845391000000	0.419857000000	-0.601630000000
C	-4.771922000000	0.737797000000	0.106409000000
H	1.405170000000	-2.128489000000	-0.645241000000
H	-0.033547000000	-0.429503000000	-1.730059000000
H	-3.419843000000	-1.867048000000	0.492877000000
H	-1.989570000000	-3.561230000000	1.584281000000
H	0.437230000000	-3.704429000000	1.019443000000
H	-3.055630000000	-0.427430000000	-2.351223000000
H	-2.086662000000	0.866946000000	-1.653119000000
H	-5.579516000000	1.016921000000	0.751969000000

PrBz-2FPHA Hetero-Dimer

Pr2F1

C	0.550374000000	-1.242014000000	2.147782000000
C	-0.348354000000	-1.594579000000	3.149659000000
C	-1.463270000000	-0.795076000000	3.402146000000
C	-1.683937000000	0.360668000000	2.655091000000
C	-0.780520000000	0.686627000000	1.658479000000
C	0.350581000000	-0.085834000000	1.379843000000
C	1.269802000000	0.303690000000	0.352473000000
C	2.065321000000	0.631504000000	-0.498007000000
H	1.421236000000	-1.859119000000	1.936563000000
H	-0.180928000000	-2.498686000000	3.731351000000
H	-2.554017000000	0.992601000000	2.819847000000
H	2.765495000000	0.923894000000	-1.251503000000
C	-0.706147000000	-1.451057000000	-1.754064000000
C	-1.760028000000	-0.639271000000	-1.347258000000
C	-2.620785000000	-1.048765000000	-0.322285000000
C	-2.409442000000	-2.282895000000	0.289925000000
C	-1.350402000000	-3.097258000000	-0.116994000000
C	-0.496799000000	-2.686113000000	-1.137538000000
C	-3.748092000000	-0.112314000000	0.080073000000
C	-4.550245000000	-0.557461000000	1.220667000000
C	-5.207741000000	-0.928178000000	2.165432000000
H	-0.035400000000	-1.112602000000	-2.541804000000
H	-1.909443000000	0.333000000000	-1.818131000000
H	-3.067331000000	-2.602525000000	1.096248000000
H	-1.191013000000	-4.056511000000	0.373974000000
H	0.331983000000	-3.319626000000	-1.449603000000
H	-4.416336000000	0.033913000000	-0.779597000000
H	-3.322159000000	0.874545000000	0.309754000000
H	-5.806271000000	-1.250653000000	2.991067000000
F	-1.011251000000	1.783578000000	0.912500000000
H	-2.174455000000	-1.073122000000	4.177696000000

Pr2F2

C	1.850667000000	-1.689708000000	0.532465000000
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C	1.869947000000	-1.942383000000	1.898916000000
C	1.034465000000	-1.222677000000	2.756081000000
C	0.185207000000	-0.241526000000	2.252316000000
C	0.185503000000	-0.004045000000	0.887567000000
C	0.994087000000	-0.714888000000	-0.002676000000
C	0.945035000000	-0.447216000000	-1.409397000000
C	0.912159000000	-0.224240000000	-2.598047000000
H	2.539882000000	-2.700787000000	2.298535000000
H	-0.456690000000	0.355007000000	2.895918000000
H	0.883795000000	-0.030417000000	-3.649340000000
C	1.356987000000	2.935179000000	3.296162000000
C	1.599956000000	2.908186000000	1.926472000000
C	2.612467000000	2.098922000000	1.396182000000
C	3.374758000000	1.315499000000	2.260632000000
C	3.133834000000	1.343545000000	3.636227000000
C	2.127243000000	2.151038000000	4.158882000000
C	2.838543000000	2.123027000000	-0.106074000000
C	3.831201000000	1.165779000000	-0.594836000000
C	4.657767000000	0.375539000000	-0.987165000000
H	0.565812000000	3.569605000000	3.693658000000
H	0.990825000000	3.514017000000	1.254825000000
H	4.155803000000	0.674837000000	1.854830000000
H	3.737404000000	0.726097000000	4.300423000000
H	1.941492000000	2.173383000000	5.231773000000
H	3.153381000000	3.133573000000	-0.401270000000
H	1.885645000000	1.933222000000	-0.619287000000
H	5.385407000000	-0.317761000000	-1.352325000000
H	1.055667000000	-1.412278000000	3.827699000000
F	-0.611435000000	0.962910000000	0.398092000000
H	2.499322000000	-2.237117000000	-0.147766000000

Pr2F3

C	1.671224000000	0.331249000000	0.900216000000
C	0.667855000000	1.283156000000	0.985677000000
C	-0.523910000000	0.942550000000	1.624869000000
C	-0.693362000000	-0.333631000000	2.163489000000
C	0.329444000000	-1.271168000000	2.071698000000
C	1.537689000000	-0.952880000000	1.434390000000
C	2.591662000000	-1.914126000000	1.302019000000
C	3.469336000000	-2.739149000000	1.188166000000
H	0.833006000000	2.267809000000	0.553265000000
H	-1.635733000000	-0.602324000000	2.635762000000
H	4.253674000000	-3.460344000000	1.096505000000
C	0.440700000000	-2.492763000000	-1.310393000000
C	-0.334297000000	-1.339651000000	-1.417180000000
C	-1.619841000000	-1.292747000000	-0.872148000000
C	-2.126439000000	-2.422860000000	-0.228026000000
C	-1.353497000000	-3.578950000000	-0.122453000000
C	-0.065871000000	-3.615841000000	-0.657369000000
C	-2.435028000000	-0.019000000000	-1.017147000000
C	-3.448915000000	0.172814000000	0.023104000000
C	-4.286093000000	0.325030000000	0.882494000000
H	1.451404000000	-2.506142000000	-1.715507000000
H	0.073827000000	-0.457837000000	-1.912444000000
H	-3.123134000000	-2.389301000000	0.210206000000
H	-1.757081000000	-4.452855000000	0.387328000000
H	0.545080000000	-4.511566000000	-0.558027000000
H	-2.935075000000	-0.012328000000	-1.996160000000
H	-1.753565000000	0.841307000000	-1.004531000000
H	-5.035295000000	0.466727000000	1.632614000000
H	-1.331210000000	1.670472000000	1.689438000000
H	0.203209000000	-2.274695000000	2.472109000000

F 2.813704000000 0.651218000000 0.267189000000

Pr2F4

C 0.612931000000 -0.913346000000 1.637542000000
C -0.325706000000 -1.560386000000 2.423529000000
C -1.416636000000 -0.833993000000 2.895897000000
C -1.547623000000 0.522325000000 2.591400000000
C -0.592646000000 1.152925000000 1.801198000000
C 0.506665000000 0.438757000000 1.299913000000
C 1.471179000000 1.051423000000 0.436068000000
C 2.270540000000 1.562467000000 -0.315011000000
H -0.202769000000 -2.620589000000 2.631832000000
H -2.406809000000 1.080249000000 2.958894000000
H 2.986835000000 2.018608000000 -0.965161000000
C -0.572199000000 -1.905884000000 -1.227214000000
C -1.556064000000 -0.967954000000 -0.919052000000
C -2.693547000000 -1.339069000000 -0.198209000000
C -2.839148000000 -2.668344000000 0.203740000000
C -1.858587000000 -3.609746000000 -0.107719000000
C -0.720414000000 -3.231201000000 -0.819831000000
C -3.751879000000 -0.291022000000 0.101118000000
C -4.548814000000 -0.560479000000 1.300731000000
C -5.202842000000 -0.785371000000 2.292895000000
H 0.321613000000 -1.594597000000 -1.766063000000
H -1.423883000000 0.071314000000 -1.222594000000
H -3.716960000000 -2.961879000000 0.778238000000
H -1.981238000000 -4.643201000000 0.213934000000
H 0.052538000000 -3.963049000000 -1.048505000000
H -4.433739000000 -0.203738000000 -0.756863000000
H -3.263076000000 0.684455000000 0.216841000000
H -5.795250000000 -0.978526000000 3.162211000000
H -2.179632000000 -1.333301000000 3.489808000000
H -0.684556000000 2.207580000000 1.548439000000
F 1.655392000000 -1.614149000000 1.162536000000

Pr2F5

C -5.199900000000 1.259313000000 8.035397000000
C -5.636198000000 0.441444000000 9.063612000000
C -6.858274000000 0.727766000000 9.670307000000
C -7.616711000000 1.818922000000 9.244928000000
C -7.160388000000 2.622244000000 8.205027000000
C -5.939018000000 2.350618000000 7.571791000000
C -5.453890000000 3.156447000000 6.491402000000
C -5.057765000000 3.840914000000 5.575630000000
H -5.015718000000 -0.394770000000 9.378070000000
H -8.566457000000 2.044522000000 9.725293000000
H -4.677500000000 4.451887000000 4.784084000000
C -4.366221000000 3.301680000000 10.747827000000
C -3.405710000000 3.369047000000 9.741164000000
C -3.441377000000 4.389807000000 8.786638000000
C -4.447231000000 5.353282000000 8.863295000000
C -5.409173000000 5.289105000000 9.872006000000
C -5.374885000000 4.262762000000 10.814658000000
C -2.400013000000 4.371494000000 7.680559000000
C -2.428447000000 5.526625000000 6.782533000000
C -2.451987000000 6.487336000000 6.048339000000
H -4.332052000000 2.493362000000 11.476872000000
H -2.626452000000 2.607863000000 9.682895000000
H -4.485041000000 6.147290000000 8.119593000000
H -6.191649000000 6.045354000000 9.918077000000
H -6.131879000000 4.208533000000 11.595497000000
H -2.545492000000 3.460552000000 7.082998000000

H	-1.399563000000	4.302234000000	8.127957000000
H	-2.455876000000	7.336924000000	5.398962000000
H	-7.215939000000	0.095531000000	10.481165000000
F	-4.007352000000	1.003542000000	7.466568000000
H	-7.739527000000	3.478558000000	7.866055000000

Pr2F6

C	-0.945245000000	0.030356000000	2.368232000000
C	0.061355000000	0.641552000000	1.627060000000
C	1.128748000000	-0.114358000000	1.138551000000
C	1.200951000000	-1.481643000000	1.397286000000
C	0.191888000000	-2.068533000000	2.141735000000
C	-0.898362000000	-1.345678000000	2.635431000000
C	-1.936313000000	-2.007890000000	3.367102000000
C	-2.815004000000	-2.573202000000	3.977346000000
H	-1.793286000000	0.601663000000	2.738795000000
H	0.012704000000	1.710550000000	1.428627000000
H	2.012141000000	-2.100584000000	1.021399000000
H	-3.583405000000	-3.073766000000	4.527359000000
C	0.356883000000	-2.339184000000	-1.976825000000
C	-0.510684000000	-1.272970000000	-1.756551000000
C	-1.615814000000	-1.414064000000	-0.910399000000
C	-1.839149000000	-2.641907000000	-0.287314000000
C	-0.970384000000	-3.712804000000	-0.506476000000
C	0.128715000000	-3.565627000000	-1.349287000000
C	-2.537707000000	-0.219853000000	-0.723252000000
C	-3.539798000000	-0.378952000000	0.331246000000
C	-4.356936000000	-0.534537000000	1.208410000000
H	1.213788000000	-2.213760000000	-2.637559000000
H	-0.326486000000	-0.314272000000	-2.243504000000
H	-2.685507000000	-2.755329000000	0.389074000000
H	-1.149102000000	-4.661149000000	-0.002787000000
H	0.807105000000	-4.400874000000	-1.516733000000
H	-3.052902000000	-0.011322000000	-1.671205000000
H	-1.927341000000	0.664473000000	-0.496087000000
H	-5.075440000000	-0.668114000000	1.989060000000
F	0.250733000000	-3.387498000000	2.385279000000
H	1.910942000000	0.360737000000	0.549086000000

Pr2F7

C	1.698663000000	0.287268000000	0.894687000000
C	0.680671000000	1.231818000000	0.971433000000
C	-0.525486000000	0.910837000000	1.598301000000
C	-0.715058000000	-0.354032000000	2.149952000000
C	0.313598000000	-1.279362000000	2.066897000000
C	1.531126000000	-0.993275000000	1.443134000000
C	2.560181000000	-1.986113000000	1.354492000000
C	3.435775000000	-2.816199000000	1.263417000000
H	0.828791000000	2.221400000000	0.543284000000
H	-1.652097000000	-0.638649000000	2.623138000000
H	4.210990000000	-3.549809000000	1.196027000000
C	0.439130000000	-2.418644000000	-1.373005000000
C	-0.369148000000	-1.288427000000	-1.480381000000
C	-1.635733000000	-1.262353000000	-0.892349000000
C	-2.089844000000	-2.390072000000	-0.205649000000
C	-1.283178000000	-3.522242000000	-0.099151000000
C	-0.014261000000	-3.538292000000	-0.676831000000
C	-2.483692000000	-0.009047000000	-1.028298000000
C	-3.476642000000	0.169329000000	0.034413000000
C	-4.294934000000	0.310542000000	0.913750000000
H	1.436145000000	-2.416457000000	-1.811378000000
H	-0.001438000000	-0.406829000000	-2.006405000000

H	-3.070124000000	-2.371045000000	0.268845000000
H	-1.640227000000	-4.388918000000	0.454722000000
H	0.626146000000	-4.412008000000	-0.570343000000
H	-3.006615000000	-0.020628000000	-1.995209000000
H	-1.821619000000	0.866663000000	-1.037959000000
H	-5.029131000000	0.441325000000	1.680528000000
H	-1.332537000000	1.640016000000	1.650536000000
F	0.134497000000	-2.496058000000	2.603970000000
H	2.641593000000	0.522162000000	0.405061000000

Pr2F8

C	-1.007583000000	0.161723000000	2.786525000000
C	-0.193203000000	1.178015000000	2.313379000000
C	0.893986000000	0.842488000000	1.505884000000
C	1.145054000000	-0.491440000000	1.179420000000
C	0.311204000000	-1.496151000000	1.660833000000
C	-0.783871000000	-1.184664000000	2.480160000000
C	-1.656494000000	-2.200762000000	2.988070000000
C	-2.384008000000	-3.067153000000	3.416487000000
H	-0.418987000000	2.207369000000	2.582319000000
H	1.985932000000	-0.750968000000	0.539646000000
H	-3.026124000000	-3.830871000000	3.801187000000
C	0.155736000000	-3.171283000000	-1.915994000000
C	-0.398091000000	-1.909070000000	-1.724509000000
C	-1.528893000000	-1.739307000000	-0.917659000000
C	-2.108603000000	-2.856729000000	-0.320431000000
C	-1.553153000000	-4.124477000000	-0.508596000000
C	-0.419622000000	-4.286715000000	-1.301385000000
C	-2.044422000000	-0.328381000000	-0.692201000000
C	-3.152102000000	-0.221912000000	0.257831000000
C	-4.048898000000	-0.151276000000	1.065195000000
H	1.039045000000	-3.287887000000	-2.542610000000
H	0.062776000000	-1.037306000000	-2.191347000000
H	-2.979943000000	-2.731607000000	0.319558000000
H	-2.007813000000	-4.987479000000	-0.023956000000
H	0.014441000000	-5.275115000000	-1.444420000000
H	-2.351541000000	0.105937000000	-1.653290000000
H	-1.211768000000	0.286752000000	-0.319987000000
H	-4.830714000000	-0.077776000000	1.791146000000
H	1.544363000000	1.630145000000	1.129485000000
H	0.479322000000	-2.537214000000	1.389291000000
F	-2.047817000000	0.479216000000	3.570836000000

Pr2F9

C	2.689073000000	-1.965665000000	0.757184000000
C	2.945145000000	-2.151575000000	2.106051000000
C	2.044135000000	-1.637165000000	3.036838000000
C	0.909387000000	-0.945374000000	2.613199000000
C	0.671584000000	-0.770220000000	1.254846000000
C	1.561027000000	-1.280600000000	0.296371000000
C	1.330889000000	-1.102751000000	-1.106574000000
C	1.124388000000	-0.928350000000	-2.285949000000
H	3.839981000000	-2.692667000000	2.405296000000
H	0.218946000000	-0.527029000000	3.342151000000
H	-0.206188000000	-0.226738000000	0.910316000000
H	0.949021000000	-0.788286000000	-3.331500000000
C	1.193946000000	2.657295000000	3.311350000000
C	1.443689000000	2.570421000000	1.945349000000
C	2.603693000000	1.948539000000	1.467285000000
C	3.511615000000	1.419190000000	2.381874000000
C	3.265483000000	1.509587000000	3.753944000000
C	2.108489000000	2.124931000000	4.223765000000

C	2.827971000000	1.891242000000	-0.034299000000
C	3.928277000000	1.023760000000	-0.455078000000
C	4.830140000000	0.292039000000	-0.789815000000
H	0.286046000000	3.142647000000	3.667263000000
H	0.726528000000	2.985128000000	1.235556000000
H	4.410218000000	0.923518000000	2.018305000000
H	3.983548000000	1.090307000000	4.457753000000
H	1.917417000000	2.193681000000	5.293693000000
H	3.014071000000	2.907983000000	-0.407712000000
H	1.908483000000	1.541259000000	-0.523644000000
H	5.609464000000	-0.370225000000	-1.102300000000
H	2.238085000000	-1.767535000000	4.099959000000
F	3.548717000000	-2.473787000000	-0.139697000000

Pr2F10

C	1.461257000000	0.683081000000	0.756373000000
C	2.212920000000	-0.479745000000	0.771271000000
C	1.679760000000	-1.611578000000	1.387134000000
C	0.417494000000	-1.564417000000	1.978455000000
C	-0.318090000000	-0.384237000000	1.958600000000
C	0.193932000000	0.767531000000	1.341673000000
C	-0.557244000000	1.987125000000	1.292413000000
C	-1.217335000000	2.999717000000	1.238770000000
H	3.192568000000	-0.484699000000	0.298448000000
H	-0.002280000000	-2.454248000000	2.442191000000
H	-1.795596000000	3.898579000000	1.202343000000
C	0.334690000000	-2.587023000000	-1.616967000000
C	-0.436963000000	-1.433250000000	-1.498394000000
C	-1.661818000000	-1.462491000000	-0.826748000000
C	-2.104683000000	-2.665839000000	-0.274712000000
C	-1.333934000000	-3.822427000000	-0.393412000000
C	-0.111995000000	-3.787388000000	-1.064133000000
C	-2.484300000000	-0.188229000000	-0.742112000000
C	-3.412747000000	-0.139803000000	0.389549000000
C	-4.180326000000	-0.107566000000	1.323410000000
H	1.292456000000	-2.545857000000	-2.134113000000
H	-0.076198000000	-0.493769000000	-1.918762000000
H	-3.051813000000	-2.692075000000	0.262563000000
H	-1.689943000000	-4.755309000000	0.041921000000
H	0.490563000000	-4.690110000000	-1.153541000000
H	-3.060951000000	-0.067475000000	-1.670353000000
H	-1.811201000000	0.675970000000	-0.675230000000
H	-4.863110000000	-0.064102000000	2.145357000000
H	2.251763000000	-2.537597000000	1.394295000000
H	-1.312478000000	-0.337396000000	2.397967000000
F	1.965691000000	1.773002000000	0.151771000000

Pr2F11

C	0.843573000000	0.352495000000	2.099799000000
C	-0.229246000000	-0.467306000000	2.412335000000
C	-1.438681000000	0.123783000000	2.769339000000
C	-1.558629000000	1.514817000000	2.819049000000
C	-0.469426000000	2.319234000000	2.504245000000
C	0.758547000000	1.747626000000	2.129569000000
C	1.888703000000	2.557507000000	1.782704000000
C	2.833206000000	3.253134000000	1.487129000000
H	-0.114302000000	-1.546980000000	2.330505000000
H	-2.509494000000	1.970795000000	3.085394000000
H	-0.549842000000	3.403822000000	2.531717000000
H	3.672602000000	3.864238000000	1.230166000000
C	0.617021000000	-2.415112000000	-0.699049000000
C	0.082827000000	-1.136511000000	-0.824533000000

C	-1.267764000000	-0.896451000000	-0.549805000000
C	-2.081457000000	-1.961647000000	-0.168050000000
C	-1.548363000000	-3.247037000000	-0.043807000000
C	-0.199181000000	-3.477527000000	-0.303522000000
C	-1.770291000000	0.534325000000	-0.634437000000
C	-3.163046000000	0.724636000000	-0.228385000000
C	-4.313890000000	0.872155000000	0.112233000000
H	1.674250000000	-2.581981000000	-0.899289000000
H	0.729873000000	-0.304991000000	-1.107796000000
H	-3.133188000000	-1.782271000000	0.049398000000
H	-2.193133000000	-4.070897000000	0.259532000000
H	0.216554000000	-4.478612000000	-0.200201000000
H	-1.647846000000	0.902919000000	-1.661862000000
H	-1.133213000000	1.164413000000	0.003629000000
H	-5.333584000000	1.016934000000	0.400370000000
H	-2.298436000000	-0.506821000000	2.988046000000
F	2.005943000000	-0.212943000000	1.734564000000

Pr2F12

C	5.930348000000	2.383911000000	-0.594688000000
C	6.033061000000	3.671312000000	-0.075586000000
C	5.898660000000	3.884347000000	1.298167000000
C	5.656825000000	2.813528000000	2.156584000000
C	5.555823000000	1.540335000000	1.618456000000
C	5.691661000000	1.288656000000	0.249222000000
C	5.601898000000	-0.046141000000	-0.263024000000
C	5.550717000000	-1.169164000000	-0.709716000000
H	6.034825000000	2.202937000000	-1.662351000000
H	6.219688000000	4.509513000000	-0.743803000000
H	5.516319000000	2.952362000000	3.227235000000
H	5.505781000000	-2.162974000000	-1.102226000000
C	2.880946000000	4.776255000000	4.111051000000
C	2.664787000000	4.445788000000	2.776636000000
C	2.526205000000	3.109621000000	2.384305000000
C	2.586646000000	2.109566000000	3.353040000000
C	2.802301000000	2.438482000000	4.693476000000
C	2.955470000000	3.768842000000	5.076696000000
C	2.372996000000	2.809810000000	0.903329000000
C	2.280285000000	1.388443000000	0.570540000000
C	2.228288000000	0.208918000000	0.312063000000
H	2.992133000000	5.820240000000	4.401371000000
H	2.620704000000	5.232889000000	2.022470000000
H	2.491684000000	1.067139000000	3.054395000000
H	2.856485000000	1.646791000000	5.439351000000
H	3.127582000000	4.023438000000	6.121370000000
H	3.240795000000	3.232253000000	0.374386000000
H	1.485534000000	3.328683000000	0.516728000000
H	2.198174000000	-0.831523000000	0.067610000000
F	5.316023000000	0.507838000000	2.440819000000
H	5.970643000000	4.890430000000	1.707579000000

Pr2F13

C	1.844079000000	0.546786000000	0.710787000000
C	2.475464000000	-0.682842000000	0.855859000000
C	1.811217000000	-1.740214000000	1.481321000000
C	0.517507000000	-1.571532000000	1.967108000000
C	-0.092538000000	-0.337432000000	1.814171000000
C	0.538581000000	0.741428000000	1.188377000000
C	-0.140332000000	1.993232000000	1.027321000000
C	-0.715816000000	3.047013000000	0.875801000000
H	2.347689000000	1.378875000000	0.223010000000
H	3.486533000000	-0.819289000000	0.477833000000

H	-0.033094000000	-2.379864000000	2.442155000000
H	-1.221928000000	3.981542000000	0.754736000000
C	0.215805000000	-2.225971000000	-1.542133000000
C	-0.679355000000	-1.178305000000	-1.353411000000
C	-1.871223000000	-1.373601000000	-0.644367000000
C	-2.149749000000	-2.636974000000	-0.126095000000
C	-1.252386000000	-3.691645000000	-0.316189000000
C	-0.070409000000	-3.491566000000	-1.023817000000
C	-2.801602000000	-0.186011000000	-0.466959000000
C	-4.012507000000	-0.461561000000	0.306088000000
C	-5.012152000000	-0.703163000000	0.941017000000
H	1.141848000000	-2.055360000000	-2.089267000000
H	-0.449223000000	-0.188215000000	-1.749850000000
H	-3.072149000000	-2.795368000000	0.430039000000
H	-1.484559000000	-4.675287000000	0.090255000000
H	0.627439000000	-4.314581000000	-1.171216000000
H	-3.094522000000	0.186225000000	-1.458239000000
H	-2.251105000000	0.630260000000	0.021123000000
H	-5.898709000000	-0.900120000000	1.505623000000
F	-1.345946000000	-0.175136000000	2.267382000000
H	2.298808000000	-2.708054000000	1.583014000000

Pr2F14

C	-0.055718000000	3.271232000000	-4.601558000000
C	-0.615437000000	3.015423000000	-5.842725000000
C	-1.012063000000	1.712159000000	-6.140823000000
C	-0.846581000000	0.693411000000	-5.201707000000
C	-0.281947000000	0.971306000000	-3.961467000000
C	0.127663000000	2.273806000000	-3.638351000000
C	0.702154000000	2.583971000000	-2.362576000000
C	1.162096000000	2.838413000000	-1.272789000000
H	-0.730743000000	3.832234000000	-6.551836000000
H	-1.163814000000	-0.321902000000	-5.431326000000
H	-0.162190000000	0.186661000000	-3.216551000000
H	1.550382000000	3.068053000000	-0.303137000000
C	-2.903469000000	-0.849729000000	-2.555144000000
C	-2.996728000000	0.452285000000	-2.069050000000
C	-2.127103000000	0.907462000000	-1.072985000000
C	-1.161363000000	0.035607000000	-0.568062000000
C	-1.063808000000	-1.268920000000	-1.055123000000
C	-1.932857000000	-1.716214000000	-2.049976000000
C	-2.242517000000	2.348985000000	-0.607948000000
C	-1.571372000000	2.638191000000	0.660175000000
C	-1.025497000000	2.864351000000	1.715175000000
H	-3.588975000000	-1.188342000000	-3.330757000000
H	-3.751370000000	1.127831000000	-2.473053000000
H	-0.482155000000	0.382507000000	0.208685000000
H	-0.306389000000	-1.939212000000	-0.651646000000
H	-1.858827000000	-2.735842000000	-2.424963000000
H	-3.303686000000	2.610772000000	-0.508599000000
H	-1.821491000000	3.006976000000	-1.381843000000
H	-0.556798000000	3.077318000000	2.652573000000
H	-1.453191000000	1.496125000000	-7.112466000000
F	0.324988000000	4.526590000000	-4.310486000000

Pr2F15

C	-0.768951000000	-0.469453000000	2.082713000000
C	-0.218283000000	0.439906000000	1.187129000000
C	1.067764000000	0.234502000000	0.683228000000
C	1.802804000000	-0.885367000000	1.064888000000
C	1.231904000000	-1.780898000000	1.953826000000
C	-0.045833000000	-1.601352000000	2.490143000000

C	-0.590170000000	-2.541432000000	3.423748000000
C	-1.074871000000	-3.327841000000	4.204618000000
H	-1.769305000000	-0.324495000000	2.485828000000
H	-0.790693000000	1.313935000000	0.883240000000
H	2.801556000000	-1.080931000000	0.681347000000
H	-1.511472000000	-4.026966000000	4.885802000000
C	-3.939533000000	-5.009704000000	2.535914000000
C	-2.763476000000	-5.113350000000	1.799071000000
C	-2.305001000000	-4.037775000000	1.031727000000
C	-3.053936000000	-2.863049000000	0.996565000000
C	-4.231670000000	-2.754615000000	1.738933000000
C	-4.675447000000	-3.822802000000	2.514458000000
C	-0.973151000000	-4.177368000000	0.315882000000
C	-0.662470000000	-3.091554000000	-0.614668000000
C	-0.422778000000	-2.184957000000	-1.377581000000
H	-4.284668000000	-5.855525000000	3.129428000000
H	-2.183566000000	-6.036646000000	1.829522000000
H	-2.706908000000	-2.026718000000	0.391466000000
H	-4.806057000000	-1.829482000000	1.707708000000
H	-5.594156000000	-3.737524000000	3.092856000000
H	-0.952407000000	-5.129532000000	-0.230148000000
H	-0.175805000000	-4.233070000000	1.072874000000
H	-0.197531000000	-1.389230000000	-2.055115000000
H	1.501666000000	0.948083000000	-0.015288000000
F	1.931903000000	-2.871595000000	2.313546000000

Pr2F16

C	6.125862000000	1.694994000000	1.676355000000
C	6.248133000000	1.625600000000	0.296526000000
C	6.459422000000	2.802382000000	-0.417958000000
C	6.543009000000	4.026860000000	0.250901000000
C	6.420413000000	4.074053000000	1.635707000000
C	6.211059000000	2.900866000000	2.378156000000
C	6.084647000000	2.931672000000	3.803967000000
C	5.980061000000	2.977635000000	5.007693000000
H	6.158238000000	0.659540000000	-0.193913000000
H	6.705405000000	4.945194000000	-0.309407000000
H	6.482694000000	5.019658000000	2.170395000000
H	5.874216000000	3.012319000000	6.071012000000
C	2.747422000000	4.563725000000	4.324479000000
C	2.891487000000	4.308301000000	2.964876000000
C	2.835586000000	2.998444000000	2.473427000000
C	2.647583000000	1.947296000000	3.368878000000
C	2.500985000000	2.202165000000	4.734299000000
C	2.544482000000	3.507420000000	5.215600000000
C	2.971172000000	2.789512000000	0.974221000000
C	2.919257000000	1.393839000000	0.538224000000
C	2.863521000000	0.237611000000	0.189038000000
H	2.790987000000	5.588165000000	4.691751000000
H	3.048027000000	5.134775000000	2.270054000000
H	2.616398000000	0.924584000000	2.997509000000
H	2.352573000000	1.371351000000	5.422688000000
H	2.426571000000	3.704771000000	6.280226000000
H	3.917772000000	3.231503000000	0.632714000000
H	2.169087000000	3.342231000000	0.466162000000
H	2.812162000000	-0.783439000000	-0.124750000000
H	6.552477000000	2.763240000000	-1.501540000000
F	5.915359000000	0.563256000000	2.363846000000

Pr2F17

C	0.886770000000	0.403940000000	2.117246000000
C	-0.201066000000	-0.415536000000	2.397952000000

C	-1.431000000000	0.149677000000	2.736776000000
C	-1.576359000000	1.534829000000	2.805041000000
C	-0.478729000000	2.333116000000	2.526745000000
C	0.766585000000	1.801846000000	2.173709000000
C	1.873203000000	2.662960000000	1.878326000000
C	2.814226000000	3.378543000000	1.622034000000
H	-0.098855000000	-1.496446000000	2.316873000000
H	-2.526279000000	2.003924000000	3.050420000000
H	3.644226000000	4.016026000000	1.401333000000
C	0.564691000000	-2.517529000000	-0.814523000000
C	0.055667000000	-1.227550000000	-0.929285000000
C	-1.266387000000	-0.946230000000	-0.568183000000
C	-2.077783000000	-1.982600000000	-0.110268000000
C	-1.569636000000	-3.278908000000	0.006125000000
C	-0.247967000000	-3.550157000000	-0.339510000000
C	-1.737424000000	0.495249000000	-0.647207000000
C	-3.123335000000	0.715420000000	-0.233133000000
C	-4.268730000000	0.887431000000	0.114150000000
H	1.597610000000	-2.720467000000	-1.094221000000
H	0.697402000000	-0.419775000000	-1.283841000000
H	-3.108905000000	-1.772171000000	0.169335000000
H	-2.212925000000	-4.079549000000	0.368819000000
H	0.148017000000	-4.560181000000	-0.246146000000
H	-1.613000000000	0.862476000000	-1.674664000000
H	-1.081020000000	1.109163000000	-0.012269000000
H	-5.283362000000	1.056286000000	0.407242000000
H	-2.291285000000	-0.488961000000	2.928825000000
F	-0.614992000000	3.668169000000	2.586879000000
H	1.847307000000	-0.024275000000	1.838026000000

Pr2F18

C	3.085481000000	0.674685000000	3.073853000000
C	4.389274000000	0.211228000000	3.003399000000
C	4.794531000000	-0.472861000000	1.858048000000
C	3.898461000000	-0.680997000000	0.808456000000
C	2.594661000000	-0.205743000000	0.898597000000
C	2.162303000000	0.484645000000	2.041089000000
C	0.821027000000	0.975308000000	2.159694000000
C	-0.314872000000	1.381751000000	2.256910000000
H	5.062162000000	0.390327000000	3.839191000000
H	4.213079000000	-1.218869000000	-0.083819000000
H	1.888263000000	-0.371476000000	0.087769000000
H	-1.330039000000	1.712337000000	2.334570000000
C	1.064415000000	-2.390317000000	-1.643285000000
C	0.129724000000	-1.355902000000	-1.677107000000
C	-0.656478000000	-1.067792000000	-0.556742000000
C	-0.497628000000	-1.834976000000	0.598834000000
C	0.439347000000	-2.867784000000	0.635490000000
C	1.222840000000	-3.149115000000	-0.483083000000
C	-1.615261000000	0.108566000000	-0.618331000000
C	-2.701105000000	0.064312000000	0.362949000000
C	-3.596521000000	0.021848000000	1.174480000000
H	1.665967000000	-2.605359000000	-2.525285000000
H	0.008743000000	-0.765190000000	-2.585672000000
H	-1.103844000000	-1.613752000000	1.475440000000
H	0.559733000000	-3.453115000000	1.545584000000
H	1.953682000000	-3.955510000000	-0.451367000000
H	-2.052566000000	0.167317000000	-1.623018000000
H	-1.044096000000	1.035809000000	-0.463002000000
H	-4.396459000000	-0.015985000000	1.883557000000
F	2.692557000000	1.331995000000	4.177773000000
H	5.815963000000	-0.843328000000	1.789135000000

Pr2F19

C	-0.794616000000	-0.482202000000	2.050239000000
C	-0.245070000000	0.406193000000	1.139951000000
C	1.048535000000	0.176096000000	0.676164000000
C	1.769176000000	-0.932781000000	1.121366000000
C	1.198336000000	-1.811743000000	2.034477000000
C	-0.102025000000	-1.601920000000	2.520588000000
C	-0.702765000000	-2.490350000000	3.470127000000
C	-1.215875000000	-3.242666000000	4.266304000000
H	-0.832749000000	1.261546000000	0.813930000000
H	2.777285000000	-1.113271000000	0.754406000000
H	-1.684270000000	-3.911360000000	4.956862000000
C	-3.862719000000	-5.024197000000	2.534204000000
C	-2.724549000000	-5.131076000000	1.741089000000
C	-2.276880000000	-4.041344000000	0.987094000000
C	-2.996416000000	-2.849197000000	1.024783000000
C	-4.133929000000	-2.736571000000	1.826040000000
C	-4.568511000000	-3.819494000000	2.585043000000
C	-0.981426000000	-4.188152000000	0.208309000000
C	-0.678599000000	-3.079643000000	-0.697221000000
C	-0.440750000000	-2.157326000000	-1.441507000000
H	-4.201042000000	-5.880701000000	3.116320000000
H	-2.167443000000	-6.068495000000	1.714803000000
H	-2.657572000000	-1.998954000000	0.434979000000
H	-4.674252000000	-1.791991000000	1.861491000000
H	-5.455458000000	-3.730833000000	3.210608000000
H	-1.007652000000	-5.121467000000	-0.369190000000
H	-0.154655000000	-4.286497000000	0.928157000000
H	-0.220232000000	-1.347384000000	-2.103523000000
H	1.493857000000	0.867021000000	-0.037722000000
F	-2.037105000000	-0.251432000000	2.505247000000
H	1.752158000000	-2.676803000000	2.394351000000

PrBz-3FPHA Hetero-Dimer

Pr3F1

C	2.192317000000	-1.535114000000	0.379344000000
C	2.783416000000	-2.104197000000	1.495418000000
C	2.244773000000	-1.994568000000	2.768895000000
C	1.059591000000	-1.275096000000	2.925554000000
C	0.438494000000	-0.683732000000	1.830969000000
C	1.004585000000	-0.812988000000	0.554279000000
C	0.385866000000	-0.180020000000	-0.577432000000
C	-0.118587000000	0.372756000000	-1.529434000000
H	2.658612000000	-1.637415000000	-0.597366000000
H	0.624935000000	-1.164607000000	3.917143000000
H	-0.473586000000	-0.105059000000	1.953770000000
H	-0.578473000000	0.841830000000	-2.373448000000
C	0.896997000000	2.876344000000	2.343830000000
C	1.579173000000	2.583564000000	1.167109000000
C	2.773128000000	1.852734000000	1.197078000000
C	3.273033000000	1.421972000000	2.424545000000
C	2.591989000000	1.719754000000	3.607070000000
C	1.403893000000	2.444621000000	3.572168000000
C	3.474330000000	1.567934000000	-0.120638000000
C	4.603042000000	0.640884000000	-0.028236000000
C	5.525051000000	-0.135591000000	0.064840000000
H	-0.032735000000	3.442418000000	2.304619000000

H	1.175592000000	2.910995000000	0.208497000000
H	4.194398000000	0.842586000000	2.454984000000
H	2.993029000000	1.375600000000	4.559653000000
H	0.872745000000	2.674657000000	4.494669000000
H	3.828821000000	2.515150000000	-0.550126000000
H	2.738763000000	1.162433000000	-0.829896000000
H	6.334858000000	-0.830462000000	0.138481000000
H	2.752720000000	-2.461072000000	3.610070000000
F	3.930149000000	-2.794862000000	1.334449000000

Pr3F2

C	0.353613000000	-1.129083000000	1.833621000000
C	-0.644955000000	-1.562177000000	2.688539000000
C	-1.653182000000	-0.729925000000	3.153847000000
C	-1.647923000000	0.603026000000	2.745633000000
C	-0.661780000000	1.076977000000	1.884444000000
C	0.337666000000	0.209020000000	1.420019000000
C	1.330264000000	0.678861000000	0.493936000000
C	2.152095000000	1.068730000000	-0.304798000000
H	1.108783000000	-1.823056000000	1.474510000000
H	-0.658792000000	2.114677000000	1.558112000000
H	2.889452000000	1.418698000000	-0.995989000000
C	-0.481197000000	-1.721762000000	-1.481936000000
C	-1.489379000000	-0.828204000000	-1.130838000000
C	-2.526520000000	-1.220625000000	-0.278400000000
C	-2.539105000000	-2.524132000000	0.218557000000
C	-1.529187000000	-3.421902000000	-0.130709000000
C	-0.499208000000	-3.024744000000	-0.981204000000
C	-3.612175000000	-0.209208000000	0.050071000000
C	-4.501488000000	-0.588028000000	1.149354000000
C	-5.233077000000	-0.902086000000	2.059600000000
H	0.327269000000	-1.395118000000	-2.134114000000
H	-1.460470000000	0.194475000000	-1.509596000000
H	-3.334319000000	-2.833038000000	0.895477000000
H	-1.544607000000	-4.432867000000	0.273372000000
H	0.290042000000	-3.725166000000	-1.250172000000
H	-4.223441000000	-0.034712000000	-0.846528000000
H	-3.138103000000	0.749523000000	0.297789000000
H	-5.894066000000	-1.175372000000	2.854838000000
H	-2.428367000000	-1.129754000000	3.802854000000
H	-2.434284000000	1.270900000000	3.093443000000
F	-0.648641000000	-2.855592000000	3.068699000000

Pr3F3

C	1.723526000000	0.365118000000	0.933640000000
C	0.656917000000	1.242123000000	1.038337000000
C	-0.549641000000	0.895511000000	1.629456000000
C	-0.686438000000	-0.397732000000	2.133557000000
C	0.362185000000	-1.308602000000	2.048777000000
C	1.569905000000	-0.930429000000	1.446341000000
C	2.643393000000	-1.877419000000	1.323774000000
C	3.541943000000	-2.679995000000	1.206558000000
H	2.648835000000	0.679015000000	0.457075000000
H	0.248971000000	-2.322940000000	2.423251000000
H	4.340950000000	-3.385311000000	1.116762000000
C	0.435021000000	-2.474613000000	-1.299342000000
C	-0.339056000000	-1.320360000000	-1.402011000000
C	-1.635077000000	-1.284411000000	-0.882599000000
C	-2.153189000000	-2.426634000000	-0.268982000000
C	-1.382061000000	-3.584326000000	-0.169712000000
C	-0.083766000000	-3.610501000000	-0.679031000000
C	-2.450126000000	-0.009312000000	-1.017478000000

C	-3.457290000000	0.174187000000	0.031079000000
C	-4.286713000000	0.318762000000	0.899314000000
H	1.453816000000	-2.480491000000	-1.684011000000
H	0.077797000000	-0.428835000000	-1.871764000000
H	-3.158497000000	-2.401660000000	0.149866000000
H	-1.795249000000	-4.467740000000	0.315387000000
H	0.525415000000	-4.508044000000	-0.585078000000
H	-2.956704000000	0.002435000000	-1.993054000000
H	-1.770166000000	0.852456000000	-1.004884000000
H	-5.030327000000	0.455133000000	1.655942000000
H	-1.362948000000	1.617099000000	1.673737000000
F	0.795822000000	2.486502000000	0.530925000000
H	-1.634011000000	-0.698866000000	2.576044000000

Pr3F4

C	-0.078730000000	-0.549287000000	2.408742000000
C	1.255257000000	-0.872128000000	2.230745000000
C	2.171423000000	-0.003353000000	1.654447000000
C	1.719611000000	1.248252000000	1.236869000000
C	0.384231000000	1.608329000000	1.394146000000
C	-0.519922000000	0.708248000000	1.978531000000
C	-1.907462000000	1.057663000000	2.099997000000
C	-3.083277000000	1.341449000000	2.142507000000
H	-0.765280000000	-1.269923000000	2.844932000000
H	2.419466000000	1.948549000000	0.784468000000
H	0.029863000000	2.584227000000	1.069274000000
H	-4.122620000000	1.591318000000	2.176905000000
C	0.356310000000	-2.109480000000	-0.679729000000
C	-0.279819000000	-0.940499000000	-1.088365000000
C	-1.629944000000	-0.721464000000	-0.793919000000
C	-2.333210000000	-1.691215000000	-0.080157000000
C	-1.695617000000	-2.863244000000	0.332805000000
C	-0.351707000000	-3.077565000000	0.035001000000
C	-2.261803000000	0.587869000000	-1.234022000000
C	-3.720736000000	0.637184000000	-1.130095000000
C	-4.927058000000	0.667464000000	-1.052824000000
H	1.408995000000	-2.263807000000	-0.912946000000
H	0.279901000000	-0.182782000000	-1.638237000000
H	-3.383095000000	-1.525545000000	0.155547000000
H	-2.256419000000	-3.613574000000	0.888618000000
H	0.145347000000	-3.989211000000	0.362198000000
H	-1.979135000000	0.790149000000	-2.275293000000
H	-1.843006000000	1.404010000000	-0.627107000000
H	-5.994609000000	0.701687000000	-0.998335000000
H	3.207699000000	-0.312436000000	1.537639000000
F	1.679421000000	-2.090893000000	2.621276000000

Pr3F5

C	-0.806427000000	0.033882000000	2.268942000000
C	0.135977000000	0.804899000000	1.593387000000
C	1.270237000000	0.215332000000	1.035064000000
C	1.433979000000	-1.155711000000	1.177855000000
C	0.523637000000	-1.955243000000	1.845695000000
C	-0.615124000000	-1.349795000000	2.394254000000
C	-1.592067000000	-2.156973000000	3.070626000000
C	-2.416410000000	-2.841608000000	3.633266000000
H	-1.700207000000	0.487062000000	2.690160000000
H	0.683723000000	-3.027707000000	1.918226000000
H	-3.140905000000	-3.443804000000	4.139301000000
C	0.203832000000	-2.581285000000	-1.639048000000
C	-0.583165000000	-1.441852000000	-1.488225000000
C	-1.787920000000	-1.494935000000	-0.780511000000

C	-2.198762000000	-2.709839000000	-0.230831000000
C	-1.412966000000	-3.852573000000	-0.381174000000
C	-0.209812000000	-3.792381000000	-1.083136000000
C	-2.617967000000	-0.227926000000	-0.655019000000
C	-3.608735000000	-0.259182000000	0.422510000000
C	-4.418351000000	-0.307914000000	1.319075000000
H	1.147784000000	-2.521488000000	-2.178428000000
H	-0.250360000000	-0.493661000000	-1.912245000000
H	-3.123357000000	-2.754836000000	0.342120000000
H	-1.739953000000	-4.791984000000	0.062506000000
H	0.406994000000	-4.683054000000	-1.192888000000
H	-3.136322000000	-0.036212000000	-1.605165000000
H	-1.943176000000	0.621542000000	-0.486124000000
H	-5.133902000000	-0.344708000000	2.112998000000
H	2.018336000000	0.794032000000	0.497880000000
F	2.521733000000	-1.735872000000	0.630308000000
H	-0.012510000000	1.879354000000	1.498892000000

Pr3F6

C	1.178477000000	0.617974000000	0.849152000000
C	1.820826000000	-0.616729000000	0.821995000000
C	1.285295000000	-1.712754000000	1.496330000000
C	0.098256000000	-1.536164000000	2.192216000000
C	-0.571270000000	-0.325179000000	2.245172000000
C	-0.021160000000	0.767038000000	1.561190000000
C	-0.707910000000	2.029313000000	1.566586000000
C	-1.308134000000	3.080154000000	1.549467000000
H	1.593701000000	1.473090000000	0.320739000000
H	-1.511523000000	-0.237224000000	2.782436000000
H	-1.832922000000	4.011992000000	1.546973000000
C	0.476100000000	-2.627073000000	-1.911766000000
C	-0.287977000000	-1.469730000000	-1.788095000000
C	-1.409969000000	-1.439813000000	-0.952865000000
C	-1.753311000000	-2.589543000000	-0.241178000000
C	-0.986747000000	-3.749832000000	-0.359715000000
C	0.128307000000	-3.773439000000	-1.195034000000
C	-2.221962000000	-0.157079000000	-0.879519000000
C	-3.240863000000	-0.129888000000	0.170406000000
C	-4.089400000000	-0.119689000000	1.031706000000
H	1.347095000000	-2.634367000000	-2.565908000000
H	-0.007999000000	-0.572680000000	-2.341901000000
H	-2.616366000000	-2.571523000000	0.422656000000
H	-1.261719000000	-4.636295000000	0.209824000000
H	0.724940000000	-4.679687000000	-1.288633000000
H	-2.717114000000	0.006574000000	-1.846936000000
H	-1.543360000000	0.693103000000	-0.728915000000
H	-4.842383000000	-0.095281000000	1.790742000000
H	1.757073000000	-2.692161000000	1.475027000000
H	2.745748000000	-0.733012000000	0.260137000000
F	-0.439243000000	-2.594138000000	2.831965000000

Pr3F7

C	-0.843285000000	0.031400000000	2.266105000000
C	0.113455000000	0.750973000000	1.569682000000
C	1.263263000000	0.174293000000	1.050464000000
C	1.455693000000	-1.194474000000	1.240671000000
C	0.516463000000	-1.953719000000	1.929891000000
C	-0.637505000000	-1.343231000000	2.443045000000
C	-1.621840000000	-2.130645000000	3.131598000000
C	-2.453318000000	-2.802764000000	3.698920000000
H	-1.738412000000	0.520868000000	2.640888000000
H	2.343513000000	-1.674146000000	0.833172000000

H	0.655624000000	-3.023852000000	2.061664000000
H	-3.182257000000	-3.393860000000	4.211625000000
C	0.182512000000	-2.569498000000	-1.747898000000
C	-0.593115000000	-1.428626000000	-1.555951000000
C	-1.760998000000	-1.480446000000	-0.788908000000
C	-2.140573000000	-2.694094000000	-0.214114000000
C	-1.363586000000	-3.837358000000	-0.402249000000
C	-0.201116000000	-3.780104000000	-1.169315000000
C	-2.588071000000	-0.214159000000	-0.634381000000
C	-3.586950000000	-0.269252000000	0.434290000000
C	-4.403237000000	-0.338609000000	1.323344000000
H	1.090863000000	-2.512869000000	-2.346352000000
H	-0.283928000000	-0.481632000000	-2.000172000000
H	-3.035793000000	-2.738775000000	0.403819000000
H	-1.667493000000	-4.775621000000	0.059867000000
H	0.404610000000	-4.673289000000	-1.315779000000
H	-3.100188000000	0.000179000000	-1.582935000000
H	-1.915925000000	0.633411000000	-0.444458000000
H	-5.125332000000	-0.390958000000	2.110460000000
H	1.979009000000	0.789728000000	0.510174000000
F	-0.091968000000	2.072552000000	1.376261000000

Pr3F8

C	1.179620000000	0.631772000000	0.798459000000
C	1.798262000000	-0.606408000000	0.787694000000
C	1.307467000000	-1.700530000000	1.485631000000
C	0.136259000000	-1.537407000000	2.222600000000
C	-0.519566000000	-0.309460000000	2.257055000000
C	0.001044000000	0.779524000000	1.544631000000
C	-0.687478000000	2.040801000000	1.548986000000
C	-1.290656000000	3.089953000000	1.530789000000
H	1.598388000000	1.460586000000	0.232951000000
H	-0.277925000000	-2.385743000000	2.763937000000
H	-1.445107000000	-0.186361000000	2.813031000000
H	-1.818334000000	4.020159000000	1.529095000000
C	0.530266000000	-2.564123000000	-1.817304000000
C	-0.249301000000	-1.418139000000	-1.677940000000
C	-1.432814000000	-1.443983000000	-0.933814000000
C	-1.827804000000	-2.640549000000	-0.333777000000
C	-1.051164000000	-3.791152000000	-0.474286000000
C	0.130032000000	-3.756903000000	-1.213941000000
C	-2.262530000000	-0.174468000000	-0.840001000000
C	-3.263716000000	-0.171691000000	0.227772000000
C	-4.099558000000	-0.179565000000	1.101470000000
H	1.455805000000	-2.522929000000	-2.389578000000
H	0.072189000000	-0.485364000000	-2.143029000000
H	-2.743123000000	-2.666160000000	0.255741000000
H	-1.371041000000	-4.718720000000	-0.001153000000
H	0.737153000000	-4.654673000000	-1.320349000000
H	-2.777757000000	-0.012385000000	-1.797495000000
H	-1.595757000000	0.685317000000	-0.694981000000
H	-4.841059000000	-0.169419000000	1.871999000000
F	2.916825000000	-0.759048000000	0.048576000000
H	1.825776000000	-2.654570000000	1.426299000000

Pr3F9

C	-5.341657000000	1.528032000000	8.220382000000
C	-5.978416000000	0.951797000000	9.305830000000
C	-7.300956000000	1.216282000000	9.631050000000
C	-8.011662000000	2.104994000000	8.824333000000
C	-7.403883000000	2.710623000000	7.728530000000
C	-6.064471000000	2.425529000000	7.425197000000

C	-5.415249000000	3.082255000000	6.324941000000
C	-4.868293000000	3.671377000000	5.419747000000
H	-4.298501000000	1.302868000000	8.014637000000
H	-7.953266000000	3.411568000000	7.104571000000
H	-4.375153000000	4.201771000000	4.632091000000
C	-3.709924000000	3.053367000000	10.877839000000
C	-2.869656000000	3.345838000000	9.806708000000
C	-3.250843000000	4.274113000000	8.831087000000
C	-4.484327000000	4.913139000000	8.949767000000
C	-5.331695000000	4.616343000000	10.018792000000
C	-4.949032000000	3.687524000000	10.984200000000
C	-2.321797000000	4.510238000000	7.652105000000
C	-2.612729000000	5.711141000000	6.867072000000
C	-2.854412000000	6.707094000000	6.225419000000
H	-3.402215000000	2.324139000000	11.625597000000
H	-1.903928000000	2.845247000000	9.724559000000
H	-4.788664000000	5.633521000000	8.192074000000
H	-6.298492000000	5.112143000000	10.093035000000
H	-5.613114000000	3.454994000000	11.815269000000
H	-2.374209000000	3.639131000000	6.982473000000
H	-1.287117000000	4.570764000000	8.013926000000
H	-3.057348000000	7.591466000000	5.659256000000
H	-7.749926000000	0.735943000000	10.497472000000
F	-5.276086000000	0.106885000000	10.088150000000
H	-9.051123000000	2.328367000000	9.058009000000

Pr3F10

C	0.323931000000	-1.097239000000	1.901025000000
C	-0.725653000000	-1.452038000000	2.742520000000
C	-1.689380000000	-0.515487000000	3.116792000000
C	-1.566707000000	0.777252000000	2.628669000000
C	-0.538078000000	1.170271000000	1.788481000000
C	0.417815000000	0.214823000000	1.416968000000
C	1.472145000000	0.577191000000	0.511342000000
C	2.347681000000	0.874966000000	-0.269834000000
H	1.062143000000	-1.833009000000	1.591900000000
H	-0.806357000000	-2.476355000000	3.100948000000
H	-0.485745000000	2.193535000000	1.424496000000
H	3.131543000000	1.142621000000	-0.946556000000
C	-0.507228000000	-1.608377000000	-1.448382000000
C	-1.534130000000	-0.767898000000	-1.025188000000
C	-2.578301000000	-1.256974000000	-0.234493000000
C	-2.582104000000	-2.606172000000	0.122191000000
C	-1.555904000000	-3.451149000000	-0.301773000000
C	-0.515042000000	-2.955614000000	-1.085806000000
C	-3.685586000000	-0.302456000000	0.181500000000
C	-4.550380000000	-0.794649000000	1.255225000000
C	-5.269118000000	-1.210192000000	2.134252000000
H	0.307790000000	-1.205583000000	-2.047556000000
H	-1.513381000000	0.288248000000	-1.297557000000
H	-3.387176000000	-2.992824000000	0.745265000000
H	-1.570024000000	-4.502085000000	-0.015640000000
H	0.287683000000	-3.615049000000	-1.412319000000
H	-4.313098000000	-0.077085000000	-0.692304000000
H	-3.240465000000	0.649721000000	0.498411000000
H	-5.915150000000	-1.562546000000	2.910347000000
F	-2.500889000000	1.691024000000	2.967557000000
H	-2.531585000000	-0.771997000000	3.754344000000

Pr3F11

C	-3.191817000000	-0.825987000000	2.952064000000
C	-2.756846000000	0.473631000000	3.197773000000

C	-3.648652000000	1.544996000000	3.146711000000
C	-4.977857000000	1.278906000000	2.841282000000
C	-5.447162000000	0.002077000000	2.586574000000
C	-4.538893000000	-1.065515000000	2.646589000000
C	-4.996503000000	-2.402806000000	2.390209000000
C	-5.383389000000	-3.530673000000	2.183361000000
H	-2.490215000000	-1.657849000000	2.964736000000
H	-1.707795000000	0.656087000000	3.423455000000
H	-6.492171000000	-0.160537000000	2.335987000000
H	-5.725405000000	-4.527821000000	2.003253000000
C	-0.116706000000	-1.288156000000	0.584368000000
C	-1.143770000000	-0.438803000000	0.184429000000
C	-2.407977000000	-0.946865000000	-0.134936000000
C	-2.621581000000	-2.322016000000	-0.069706000000
C	-1.593033000000	-3.176801000000	0.333684000000
C	-0.341219000000	-2.665041000000	0.666454000000
C	-3.508662000000	0.039630000000	-0.485347000000
C	-4.809633000000	-0.564635000000	-0.772915000000
C	-5.879157000000	-1.081120000000	-0.997894000000
H	0.861019000000	-0.878393000000	0.834705000000
H	-0.971349000000	0.637435000000	0.137390000000
H	-3.604693000000	-2.724053000000	-0.306809000000
H	-1.777247000000	-4.248610000000	0.393477000000
H	0.458746000000	-3.332148000000	0.983898000000
H	-3.196849000000	0.642475000000	-1.348816000000
H	-3.627901000000	0.736653000000	0.357749000000
H	-6.829514000000	-1.528699000000	-1.198011000000
H	-3.334847000000	2.569197000000	3.335734000000
F	-5.846437000000	2.309529000000	2.785742000000

Pr3F12

C	-5.365255000000	1.492888000000	8.208524000000
C	-5.991238000000	0.883054000000	9.291334000000
C	-7.315632000000	1.181303000000	9.608971000000
C	-7.987094000000	2.101564000000	8.816072000000
C	-7.399735000000	2.728650000000	7.730649000000
C	-6.066983000000	2.419086000000	7.425639000000
C	-5.413939000000	3.081723000000	6.331255000000
C	-4.863310000000	3.670642000000	5.428156000000
H	-4.327169000000	1.272388000000	7.971567000000
H	-5.439003000000	0.172777000000	9.903893000000
H	-7.962487000000	3.447443000000	7.140336000000
H	-4.365675000000	4.201668000000	4.643754000000
C	-3.665075000000	3.097816000000	10.910621000000
C	-2.834776000000	3.383794000000	9.829955000000
C	-3.240785000000	4.279820000000	8.834784000000
C	-4.488233000000	4.892918000000	8.944201000000
C	-5.325969000000	4.600768000000	10.022072000000
C	-4.919325000000	3.702991000000	11.006427000000
C	-2.323203000000	4.511264000000	7.646179000000
C	-2.620562000000	5.711252000000	6.861946000000
C	-2.867243000000	6.706542000000	6.221202000000
H	-3.333596000000	2.400857000000	11.679280000000
H	-1.856279000000	2.907083000000	9.757820000000
H	-4.810503000000	5.590503000000	8.172700000000
H	-6.303161000000	5.076802000000	10.089438000000
H	-5.575400000000	3.474950000000	11.845019000000
H	-2.384352000000	3.638702000000	6.979195000000
H	-1.285011000000	4.571417000000	7.997325000000
H	-3.074992000000	7.590536000000	5.656147000000
H	-7.827379000000	0.720726000000	10.451008000000
F	-9.268318000000	2.401340000000	9.116463000000

Pr3F13

C	6.164710000000	1.697693000000	1.619966000000
C	6.298734000000	1.716295000000	0.233596000000
C	6.485396000000	2.918288000000	-0.447821000000
C	6.529015000000	4.091776000000	0.295169000000
C	6.399697000000	4.114105000000	1.673535000000
C	6.218522000000	2.895716000000	2.345492000000
C	6.077451000000	2.884849000000	3.774133000000
C	5.952618000000	2.876246000000	4.977285000000
H	6.000804000000	0.761960000000	2.148758000000
H	6.239796000000	0.785012000000	-0.325801000000
H	6.437545000000	5.055963000000	2.215218000000
H	5.831247000000	2.867860000000	6.039592000000
C	2.798983000000	4.608215000000	4.255300000000
C	2.945529000000	4.281781000000	2.911237000000
C	2.826418000000	2.954991000000	2.480509000000
C	2.568079000000	1.959275000000	3.420504000000
C	2.419337000000	2.285231000000	4.770700000000
C	2.529946000000	3.607438000000	5.191763000000
C	2.967110000000	2.669847000000	0.994783000000
C	2.933457000000	1.253303000000	0.629824000000
C	2.893970000000	0.080256000000	0.338469000000
H	2.894296000000	5.644913000000	4.575249000000
H	3.156912000000	5.064625000000	2.181328000000
H	2.480902000000	0.923970000000	3.095245000000
H	2.214573000000	1.497479000000	5.494550000000
H	2.411545000000	3.860677000000	6.244402000000
H	3.909479000000	3.104008000000	0.633619000000
H	2.160090000000	3.186001000000	0.456654000000
H	2.854374000000	-0.953262000000	0.066408000000
F	6.701785000000	5.261778000000	-0.354019000000
H	6.588804000000	2.960864000000	-1.529547000000

Pr3F14

C	-3.268730000000	-0.695470000000	2.659891000000
C	-3.217509000000	0.687818000000	2.617174000000
C	-4.341540000000	1.491506000000	2.738829000000
C	-5.578347000000	0.870878000000	2.910230000000
C	-5.674621000000	-0.516575000000	2.946810000000
C	-4.520918000000	-1.303756000000	2.817296000000
C	-4.618819000000	-2.736977000000	2.832337000000
C	-4.707570000000	-3.944109000000	2.839116000000
H	-2.361346000000	-1.286014000000	2.549731000000
H	-6.638838000000	-1.003775000000	3.072195000000
H	-4.784806000000	-5.010674000000	2.854753000000
C	-0.078478000000	-1.705995000000	0.663096000000
C	-0.819844000000	-0.638086000000	0.161051000000
C	-2.134712000000	-0.827166000000	-0.272841000000
C	-2.693910000000	-2.104637000000	-0.212039000000
C	-1.953325000000	-3.175121000000	0.288471000000
C	-0.645559000000	-2.979528000000	0.731269000000
C	-2.920870000000	0.370598000000	-0.778856000000
C	-4.373482000000	0.216615000000	-0.672573000000
C	-5.569745000000	0.067508000000	-0.583556000000
H	0.939849000000	-1.541690000000	1.012183000000
H	-0.383421000000	0.360452000000	0.136231000000
H	-3.728075000000	-2.254132000000	-0.518780000000
H	-2.409501000000	-4.161750000000	0.350500000000
H	-0.072056000000	-3.812989000000	1.133690000000
H	-2.660101000000	0.567016000000	-1.828505000000
H	-2.617947000000	1.258416000000	-0.207961000000

H	-6.628631000000	-0.054753000000	-0.498733000000
H	-4.239099000000	2.573518000000	2.696755000000
F	-2.016395000000	1.282509000000	2.438318000000
H	-6.475304000000	1.479560000000	3.008643000000

Pr3F15

C	6.099327000000	1.664906000000	1.756753000000
C	6.234162000000	1.553121000000	0.382289000000
C	6.462501000000	2.646533000000	-0.441975000000
C	6.568510000000	3.906356000000	0.149369000000
C	6.446637000000	4.057411000000	1.528503000000
C	6.212109000000	2.934880000000	2.337870000000
C	6.081713000000	3.081038000000	3.760131000000
C	5.969005000000	3.202931000000	4.958332000000
H	5.901949000000	0.783481000000	2.361629000000
H	6.529404000000	5.037865000000	1.991501000000
H	5.857142000000	3.310564000000	6.016207000000
C	2.661649000000	4.515312000000	4.411698000000
C	2.819278000000	4.315583000000	3.043996000000
C	2.817807000000	3.023863000000	2.504995000000
C	2.667416000000	1.934225000000	3.361289000000
C	2.511031000000	2.132294000000	4.734809000000
C	2.502436000000	3.420435000000	5.263572000000
C	2.972336000000	2.874244000000	1.001016000000
C	2.977317000000	1.495741000000	0.511150000000
C	2.987050000000	0.353866000000	0.114076000000
H	2.662497000000	5.526805000000	4.815687000000
H	2.944612000000	5.172649000000	2.380816000000
H	2.668599000000	0.925967000000	2.950202000000
H	2.391561000000	1.272189000000	5.392256000000
H	2.375016000000	3.573637000000	6.334368000000
H	3.907794000000	3.359292000000	0.688344000000
H	2.157597000000	3.419379000000	0.505212000000
H	3.012383000000	-0.649769000000	-0.254372000000
H	6.552485000000	2.501907000000	-1.516012000000
H	6.749378000000	4.778477000000	-0.476255000000
F	6.141620000000	0.332004000000	-0.175346000000

Pr3F16

C	0.888654000000	0.465015000000	2.083703000000
C	-0.144707000000	-0.423356000000	2.370236000000
C	-1.401757000000	0.047065000000	2.745501000000
C	-1.593423000000	1.419921000000	2.828183000000
C	-0.592974000000	2.335247000000	2.545491000000
C	0.667304000000	1.847971000000	2.167662000000
C	1.726263000000	2.770090000000	1.861663000000
C	2.617229000000	3.545320000000	1.597763000000
H	0.020063000000	-1.495512000000	2.272062000000
H	-0.788984000000	3.402145000000	2.614965000000
H	3.405922000000	4.231050000000	1.369682000000
C	0.524101000000	-2.653439000000	-0.822531000000
C	0.096451000000	-1.334301000000	-0.941543000000
C	-1.205597000000	-0.969367000000	-0.582048000000
C	-2.079289000000	-1.951339000000	-0.118557000000
C	-1.653046000000	-3.276255000000	0.002356000000
C	-0.351155000000	-3.631309000000	-0.343658000000
C	-1.589952000000	0.496684000000	-0.676032000000
C	-2.935880000000	0.815218000000	-0.199179000000
C	-4.048380000000	1.067992000000	0.200686000000
H	1.542266000000	-2.921360000000	-1.101726000000
H	0.786853000000	-0.569679000000	-1.300288000000
H	-3.094286000000	-1.674799000000	0.162773000000

H	-2.344646000000	-4.033608000000	0.369073000000
H	-0.019057000000	-4.663769000000	-0.246402000000
H	-1.493211000000	0.831122000000	-1.717752000000
H	-0.866066000000	1.082378000000	-0.089998000000
H	-5.024390000000	1.314187000000	0.562165000000
H	-2.230778000000	-0.625532000000	2.953452000000
F	-2.802691000000	1.883587000000	3.195659000000
H	1.867431000000	0.098601000000	1.783095000000

Pr3F17

C	5.985300000000	2.427521000000	-0.629566000000
C	6.089437000000	3.683414000000	-0.053277000000
C	5.936857000000	3.902830000000	1.309029000000
C	5.664378000000	2.805789000000	2.126510000000
C	5.552294000000	1.528719000000	1.585068000000
C	5.715764000000	1.333840000000	0.205407000000
C	5.614259000000	0.016156000000	-0.357581000000
C	5.547352000000	-1.094327000000	-0.833720000000
H	6.111972000000	2.302493000000	-1.701949000000
H	5.509257000000	2.956987000000	3.194034000000
H	5.489631000000	-2.075376000000	-1.255791000000
C	2.902350000000	4.788422000000	4.086251000000
C	2.705947000000	4.417881000000	2.759094000000
C	2.524179000000	3.075063000000	2.410873000000
C	2.520768000000	2.110278000000	3.416701000000
C	2.717032000000	2.478897000000	4.749802000000
C	2.914033000000	3.815610000000	5.088897000000
C	2.386925000000	2.728335000000	0.938957000000
C	2.271907000000	1.299143000000	0.649110000000
C	2.196620000000	0.115586000000	0.415375000000
H	3.047893000000	5.837266000000	4.341465000000
H	2.712497000000	5.177789000000	1.976454000000
H	2.379922000000	1.063272000000	3.152827000000
H	2.716280000000	1.714800000000	5.526003000000
H	3.070305000000	4.101580000000	6.127876000000
H	3.268509000000	3.118287000000	0.408483000000
H	1.514084000000	3.249112000000	0.522709000000
H	2.141012000000	-0.927656000000	0.187631000000
H	6.020513000000	4.911588000000	1.707302000000
H	5.321783000000	0.675771000000	2.218892000000
F	6.347156000000	4.738338000000	-0.854453000000

Pr3F18

C	0.203822000000	-0.384128000000	1.883258000000
C	1.583941000000	-0.558425000000	1.831483000000
C	2.443677000000	0.538954000000	1.861367000000
C	1.884319000000	1.807271000000	1.941218000000
C	0.517955000000	2.022849000000	1.993732000000
C	-0.333580000000	0.908058000000	1.965414000000
C	-1.757576000000	1.097377000000	2.003826000000
C	-2.957299000000	1.257995000000	2.005931000000
H	-0.464997000000	-1.241169000000	1.843145000000
H	0.123839000000	3.034169000000	2.057400000000
H	-4.018087000000	1.393421000000	1.989423000000
C	0.007368000000	-2.642935000000	-0.797490000000
C	-0.495390000000	-1.421540000000	-1.239441000000
C	-1.768198000000	-0.990576000000	-0.852344000000
C	-2.533519000000	-1.805064000000	-0.016720000000
C	-2.031330000000	-3.028647000000	0.429728000000
C	-0.759999000000	-3.451485000000	0.042592000000
C	-2.250569000000	0.370121000000	-1.324643000000
C	-3.692439000000	0.587407000000	-1.196949000000

C	-4.886486000000	0.752331000000	-1.101374000000
H	1.000210000000	-2.964356000000	-1.109156000000
H	0.111563000000	-0.789491000000	-1.888538000000
H	-3.525741000000	-1.476351000000	0.287357000000
H	-2.639190000000	-3.655183000000	1.080740000000
H	-0.371891000000	-4.408716000000	0.387385000000
H	-1.969381000000	0.506061000000	-2.376735000000
H	-1.728335000000	1.149523000000	-0.751047000000
H	-5.942252000000	0.908921000000	-1.032667000000
H	3.525315000000	0.429387000000	1.823031000000
F	2.706613000000	2.876877000000	1.968467000000
H	1.995236000000	-1.563928000000	1.761030000000

Pr3F19

C	3.121740000000	0.654839000000	2.991452000000
C	4.391024000000	0.091518000000	2.899479000000
C	4.777724000000	-0.607309000000	1.755618000000
C	3.863756000000	-0.720722000000	0.717396000000
C	2.593261000000	-0.173180000000	0.769718000000
C	2.218076000000	0.523172000000	1.926379000000
C	0.900964000000	1.090323000000	2.020102000000
C	-0.209959000000	1.563223000000	2.111357000000
H	2.818626000000	1.198285000000	3.883310000000
H	5.090483000000	0.195571000000	3.727114000000
H	1.906724000000	-0.299984000000	-0.064139000000
H	-1.206612000000	1.947662000000	2.182103000000
C	1.001354000000	-2.464022000000	-1.543718000000
C	0.054111000000	-1.443705000000	-1.611181000000
C	-0.695167000000	-1.089213000000	-0.483796000000
C	-0.489696000000	-1.779671000000	0.711365000000
C	0.459372000000	-2.800506000000	0.780519000000
C	1.208683000000	-3.144517000000	-0.343350000000
C	-1.666468000000	0.074044000000	-0.589748000000
C	-2.694887000000	0.112410000000	0.451699000000
C	-3.543555000000	0.139033000000	1.312723000000
H	1.582760000000	-2.723862000000	-2.426747000000
H	-0.103456000000	-0.912834000000	-2.550635000000
H	-1.067605000000	-1.508073000000	1.592961000000
H	0.617264000000	-3.324750000000	1.721721000000
H	1.955643000000	-3.934237000000	-0.285244000000
H	-2.160807000000	0.044964000000	-1.569009000000
H	-1.095589000000	1.013430000000	-0.548506000000
H	-4.303122000000	0.160937000000	2.065510000000
H	5.763155000000	-1.057572000000	1.659196000000
F	4.228077000000	-1.397195000000	-0.392047000000

Pr3F20

C	2.165053000000	0.158599000000	0.910622000000
C	1.346053000000	1.282500000000	0.863540000000
C	0.043884000000	1.233350000000	1.361898000000
C	-0.407218000000	0.036471000000	1.901234000000
C	0.380539000000	-1.099689000000	1.974639000000
C	1.683954000000	-1.035985000000	1.467410000000
C	2.519486000000	-2.204287000000	1.499450000000
C	3.223833000000	-3.188425000000	1.514563000000
H	3.178672000000	0.192541000000	0.518272000000
H	1.723489000000	2.209640000000	0.436085000000
H	-0.020864000000	-2.020369000000	2.389495000000
H	3.849704000000	-4.055477000000	1.538502000000
C	0.335960000000	-2.052400000000	-1.393608000000
C	-0.613568000000	-1.036359000000	-1.356231000000
C	-1.834551000000	-1.222825000000	-0.697026000000

C	-2.090561000000	-2.445291000000	-0.078859000000
C	-1.137971000000	-3.467182000000	-0.116668000000
C	0.075887000000	-3.275349000000	-0.770926000000
C	-2.815830000000	-0.064016000000	-0.662327000000
C	-4.098156000000	-0.354593000000	-0.020787000000
C	-5.155282000000	-0.604360000000	0.509110000000
H	1.287427000000	-1.888479000000	-1.897700000000
H	-0.401819000000	-0.078078000000	-1.832609000000
H	-3.036267000000	-2.595546000000	0.439016000000
H	-1.349606000000	-4.417896000000	0.370937000000
H	0.822897000000	-4.066856000000	-0.787945000000
H	-3.004686000000	0.276254000000	-1.689334000000
H	-2.344996000000	0.779127000000	-0.136730000000
H	-6.093826000000	-0.812374000000	0.977660000000
H	-0.616103000000	2.098187000000	1.339951000000
F	-1.674052000000	-0.026446000000	2.356840000000

Pr3F21

C	-0.781663000000	-0.606425000000	2.074661000000
C	-0.272684000000	0.316846000000	1.178196000000
C	1.019020000000	0.246404000000	0.675657000000
C	1.831460000000	-0.807292000000	1.092298000000
C	1.355699000000	-1.756790000000	1.991250000000
C	0.047362000000	-1.658807000000	2.487048000000
C	-0.454168000000	-2.633676000000	3.415050000000
C	-0.892576000000	-3.462612000000	4.180056000000
H	-1.800960000000	-0.517834000000	2.442132000000
H	1.989792000000	-2.577304000000	2.319382000000
H	-1.292071000000	-4.189660000000	4.854994000000
C	-4.008168000000	-4.935825000000	2.546209000000
C	-2.828006000000	-5.066096000000	1.820865000000
C	-2.359119000000	-4.015874000000	1.024378000000
C	-3.101582000000	-2.839072000000	0.950696000000
C	-4.284382000000	-2.703709000000	1.681579000000
C	-4.738808000000	-3.746852000000	2.484098000000
C	-1.030947000000	-4.191944000000	0.309281000000
C	-0.680312000000	-3.111341000000	-0.612824000000
C	-0.407052000000	-2.212447000000	-1.373555000000
H	-4.361429000000	-5.762195000000	3.161901000000
H	-2.253430000000	-5.991466000000	1.880814000000
H	-2.748993000000	-2.022659000000	0.322112000000
H	-4.854092000000	-1.777362000000	1.618082000000
H	-5.661325000000	-3.640643000000	3.052831000000
H	-1.040916000000	-5.140432000000	-0.243759000000
H	-0.238878000000	-4.277930000000	1.068158000000
H	-0.156126000000	-1.422139000000	-2.048662000000
H	1.366430000000	1.001921000000	-0.025686000000
F	-1.069756000000	1.327313000000	0.772704000000
H	2.846709000000	-0.887172000000	0.708252000000

Pr3F22

C	3.167676000000	0.736967000000	2.984321000000
C	4.439015000000	0.207021000000	2.845343000000
C	4.831536000000	-0.527752000000	1.734737000000
C	3.897582000000	-0.735057000000	0.720106000000
C	2.609820000000	-0.216837000000	0.821195000000
C	2.240186000000	0.520153000000	1.954949000000
C	0.908863000000	1.048708000000	2.070913000000
C	-0.213162000000	1.491350000000	2.177282000000
H	2.904246000000	1.304995000000	3.873095000000
H	1.881820000000	-0.388831000000	0.032061000000
H	-1.218503000000	1.850175000000	2.259361000000

C	0.953257000000	-2.507681000000	-1.557655000000
C	0.041375000000	-1.454291000000	-1.615768000000
C	-0.704129000000	-1.093008000000	-0.488888000000
C	-0.528679000000	-1.807003000000	0.697872000000
C	0.385918000000	-2.858529000000	0.758770000000
C	1.129420000000	-3.212392000000	-0.366306000000
C	-1.636649000000	0.102342000000	-0.581552000000
C	-2.690022000000	0.137455000000	0.434901000000
C	-3.559173000000	0.161094000000	1.275303000000
H	1.522692000000	-2.780328000000	-2.445054000000
H	-0.093385000000	-0.906007000000	-2.548662000000
H	-1.104135000000	-1.529935000000	1.579369000000
H	0.519965000000	-3.401698000000	1.692791000000
H	1.842340000000	-4.033783000000	-0.315825000000
H	-2.106021000000	0.119857000000	-1.573213000000
H	-1.038717000000	1.021478000000	-0.494079000000
H	-4.337280000000	0.180821000000	2.009006000000
H	5.844293000000	-0.921103000000	1.680342000000
F	5.334151000000	0.413676000000	3.833831000000
H	4.176556000000	-1.311781000000	-0.160182000000

Pr3F23

C	-0.777534000000	-0.584613000000	2.097073000000
C	-0.304271000000	0.368137000000	1.200427000000
C	0.983587000000	0.271874000000	0.673972000000
C	1.774583000000	-0.798133000000	1.067190000000
C	1.341784000000	-1.763055000000	1.960286000000
C	0.045539000000	-1.653189000000	2.482114000000
C	-0.441053000000	-2.636929000000	3.408724000000
C	-0.868816000000	-3.473565000000	4.171403000000
H	-1.782941000000	-0.517849000000	2.506005000000
H	-0.943806000000	1.198016000000	0.905199000000
H	1.998765000000	-2.581845000000	2.243465000000
H	-1.259150000000	-4.206062000000	4.845823000000
C	-4.024586000000	-4.930641000000	2.536944000000
C	-2.839861000000	-5.070998000000	1.820959000000
C	-2.355065000000	-4.024445000000	1.029159000000
C	-3.085617000000	-2.840545000000	0.951223000000
C	-4.273235000000	-2.695388000000	1.672217000000
C	-4.744032000000	-3.735148000000	2.469707000000
C	-1.023076000000	-4.211640000000	0.324618000000
C	-0.655378000000	-3.136663000000	-0.597315000000
C	-0.361313000000	-2.243890000000	-1.357483000000
H	-4.390275000000	-5.754227000000	3.149079000000
H	-2.274446000000	-6.001759000000	1.884372000000
H	-2.717785000000	-2.026506000000	0.328410000000
H	-4.834294000000	-1.763912000000	1.605664000000
H	-5.670294000000	-3.621148000000	3.030805000000
H	-1.035092000000	-5.161531000000	-0.225895000000
H	-0.237712000000	-4.301777000000	1.090097000000
H	-0.086161000000	-1.462244000000	-2.033189000000
H	1.377830000000	1.003087000000	-0.028400000000
F	3.018773000000	-0.903939000000	0.558383000000

PrBz-4FPHA Hetero-Dimer

Pr4F1

C	6.440660000000	0.746940000000	3.529719000000
C	5.739863000000	0.001798000000	4.472883000000
C	5.260935000000	0.650113000000	5.600884000000

C	5.450402000000	2.007458000000	5.824781000000
C	6.144739000000	2.743532000000	4.873600000000
C	6.645022000000	2.120283000000	3.720029000000
C	7.323936000000	2.894986000000	2.719862000000
C	7.863262000000	3.555885000000	1.859787000000
H	6.814233000000	0.267268000000	2.627173000000
H	5.551378000000	-1.060289000000	4.335941000000
H	5.039227000000	2.470278000000	6.718832000000
H	6.288985000000	3.813244000000	5.007365000000
H	8.366855000000	4.133566000000	1.113839000000
F	4.567000000000	-0.062359000000	6.511885000000
C	3.464742000000	4.704611000000	3.506246000000
C	3.966057000000	3.954586000000	2.446897000000
C	3.700691000000	2.582735000000	2.355530000000
C	2.926994000000	1.975131000000	3.342532000000
C	2.420516000000	2.727425000000	4.405292000000
C	2.686294000000	4.091335000000	4.491215000000
C	4.271710000000	1.821599000000	1.171050000000
C	4.045386000000	0.375846000000	1.194212000000
C	3.850050000000	-0.817297000000	1.215830000000
H	3.680110000000	5.770702000000	3.564904000000
H	4.583422000000	4.432514000000	1.685521000000
H	2.724379000000	0.906906000000	3.283919000000
H	1.819729000000	2.238603000000	5.171264000000
H	2.290859000000	4.677013000000	5.319880000000
H	5.352569000000	2.013935000000	1.115523000000
H	3.839117000000	2.226201000000	0.245663000000
H	3.676361000000	-1.872632000000	1.219074000000

Pr4F2

C	7.225529000000	3.021563000000	4.688763000000
C	6.543296000000	3.194219000000	5.887815000000
C	5.446521000000	2.382519000000	6.146863000000
C	5.012846000000	1.405161000000	5.264062000000
C	5.701889000000	1.240993000000	4.067161000000
C	6.809844000000	2.047820000000	3.767655000000
C	7.502157000000	1.888189000000	2.519123000000
C	8.065534000000	1.766785000000	1.454305000000
H	8.087053000000	3.643502000000	4.454842000000
H	6.842050000000	3.946125000000	6.614825000000
H	4.137172000000	0.807938000000	5.506603000000
H	5.369934000000	0.501974000000	3.340444000000
H	8.565732000000	1.645280000000	0.516931000000
F	4.771393000000	2.561837000000	7.299287000000
C	3.384391000000	4.545727000000	4.704243000000
C	4.027263000000	4.271090000000	3.499190000000
C	3.578289000000	3.238592000000	2.672023000000
C	2.468056000000	2.488927000000	3.064417000000
C	1.821609000000	2.763961000000	4.269805000000
C	2.278958000000	3.790217000000	5.095605000000
C	4.305389000000	2.971719000000	1.365119000000
C	4.213346000000	1.586754000000	0.896756000000
C	4.130380000000	0.442005000000	0.515977000000
H	3.757069000000	5.341496000000	5.347936000000
H	4.905232000000	4.848996000000	3.208710000000
H	2.121229000000	1.673358000000	2.430989000000
H	0.959253000000	2.168873000000	4.567624000000
H	1.783688000000	3.994284000000	6.043357000000
H	5.366526000000	3.226188000000	1.482645000000
H	3.905080000000	3.631965000000	0.582453000000
H	4.067232000000	-0.567014000000	0.167231000000

Pr4F3

C	0.399392000000	-1.082441000000	1.784334000000
C	-0.472835000000	-1.614492000000	2.726557000000
C	-1.446000000000	-0.788081000000	3.271274000000
C	-1.577753000000	0.547131000000	2.915521000000
C	-0.698392000000	1.069816000000	1.972547000000
C	0.292165000000	0.260955000000	1.396590000000
C	1.170731000000	0.795480000000	0.394434000000
C	1.896686000000	1.240143000000	-0.466801000000
H	1.158641000000	-1.711453000000	1.325298000000
H	-0.418311000000	-2.657177000000	3.030693000000
H	-2.364202000000	1.148546000000	3.365256000000
H	-0.776339000000	2.112725000000	1.671233000000
H	2.551126000000	1.639037000000	-1.212642000000
F	-2.294628000000	-1.302451000000	4.182031000000
C	-0.499772000000	-1.805647000000	-1.504468000000
C	-1.451880000000	-0.860880000000	-1.130084000000
C	-2.502765000000	-1.205689000000	-0.275132000000
C	-2.588594000000	-2.515227000000	0.199444000000
C	-1.639517000000	-3.465844000000	-0.178862000000
C	-0.592691000000	-3.114865000000	-1.029883000000
C	-3.532113000000	-0.145856000000	0.081521000000
C	-4.317857000000	-0.441847000000	1.280833000000
C	-4.953779000000	-0.702594000000	2.275449000000
H	0.322858000000	-1.513772000000	-2.155590000000
H	-1.360921000000	0.165742000000	-1.487419000000
H	-3.394484000000	-2.786944000000	0.879768000000
H	-1.717443000000	-4.484854000000	0.197979000000
H	0.150089000000	-3.856510000000	-1.320221000000
H	-4.219571000000	-0.009320000000	-0.765220000000
H	-3.017606000000	0.812877000000	0.226427000000
H	-5.510864000000	-0.928102000000	3.160206000000

Pr4F4

C	-0.840586000000	-0.000354000000	2.391143000000
C	0.117338000000	0.748760000000	1.712659000000
C	1.210568000000	0.088545000000	1.170954000000
C	1.393672000000	-1.282359000000	1.290460000000
C	0.432162000000	-2.019930000000	1.969421000000
C	-0.694360000000	-1.388222000000	2.518709000000
C	-1.701100000000	-2.167000000000	3.182952000000
C	-2.553358000000	-2.833749000000	3.726144000000
H	-1.718800000000	0.483781000000	2.811501000000
H	0.026428000000	1.826904000000	1.598923000000
H	2.264273000000	-1.753246000000	0.840105000000
H	0.536087000000	-3.098607000000	2.061732000000
H	-3.299174000000	-3.419789000000	4.219723000000
F	2.130620000000	0.807381000000	0.494280000000
C	0.266225000000	-2.474838000000	-1.782758000000
C	-0.512142000000	-1.340481000000	-1.564429000000
C	-1.685374000000	-1.415090000000	-0.807175000000
C	-2.067468000000	-2.644014000000	-0.267742000000
C	-1.288053000000	-3.780882000000	-0.482994000000
C	-0.120401000000	-3.701251000000	-1.240584000000
C	-2.515869000000	-0.154858000000	-0.626307000000
C	-3.519557000000	-0.235675000000	0.436081000000
C	-4.339740000000	-0.326711000000	1.319565000000
H	1.179058000000	-2.399882000000	-2.372174000000
H	-0.199169000000	-0.381321000000	-1.979284000000
H	-2.965994000000	-2.706209000000	0.344168000000
H	-1.594231000000	-4.732107000000	-0.049709000000
H	0.486902000000	-4.589695000000	-1.408076000000

H	-3.022996000000	0.081664000000	-1.572252000000
H	-1.843177000000	0.685821000000	-0.411902000000
H	-5.063441000000	-0.402866000000	2.103221000000

Pr4F5

C	7.395208000000	3.804629000000	3.368095000000
C	7.118144000000	3.792910000000	2.005184000000
C	6.384984000000	2.732218000000	1.489915000000
C	5.922518000000	1.687336000000	2.276717000000
C	6.204286000000	1.711766000000	3.638827000000
C	6.939192000000	2.767764000000	4.195431000000
C	7.202770000000	2.802210000000	5.606772000000
C	7.416108000000	2.840207000000	6.797932000000
H	7.964220000000	4.623382000000	3.803531000000
H	7.460069000000	4.585724000000	1.343580000000
H	5.331563000000	0.893240000000	1.825295000000
H	5.836093000000	0.919350000000	4.286546000000
H	7.614586000000	2.866264000000	7.848452000000
F	6.100753000000	2.726733000000	0.170519000000
C	4.085404000000	4.297369000000	4.979868000000
C	3.846220000000	4.304031000000	3.607882000000
C	3.163446000000	3.247594000000	2.998797000000
C	2.709900000000	2.189064000000	3.786709000000
C	2.946084000000	2.182371000000	5.162218000000
C	3.638268000000	3.232593000000	5.762600000000
C	2.933109000000	3.290567000000	1.497343000000
C	2.704379000000	1.980894000000	0.882659000000
C	2.514484000000	0.895989000000	0.383785000000
H	4.643302000000	5.113191000000	5.437634000000
H	4.217893000000	5.127407000000	2.996839000000
H	2.187513000000	1.356555000000	3.317482000000
H	2.593160000000	1.346977000000	5.765594000000
H	3.842788000000	3.216865000000	6.831662000000
H	3.802234000000	3.754767000000	1.013204000000
H	2.070040000000	3.934980000000	1.277420000000
H	2.343241000000	-0.055585000000	-0.073472000000

Pr4F6

C	-5.341022000000	1.532292000000	8.181416000000
C	-5.961543000000	0.897987000000	9.251654000000
C	-7.282298000000	1.215691000000	9.532553000000
C	-8.006551000000	2.134128000000	8.785383000000
C	-7.375830000000	2.760936000000	7.715761000000
C	-6.039613000000	2.468461000000	7.406785000000
C	-5.378353000000	3.153414000000	6.331966000000
C	-4.820835000000	3.762798000000	5.446437000000
H	-4.299981000000	1.317797000000	7.949530000000
H	-5.434953000000	0.178300000000	9.874246000000
H	-9.040870000000	2.346939000000	9.046246000000
H	-7.914173000000	3.490952000000	7.114962000000
H	-4.317587000000	4.311247000000	4.677967000000
F	-7.885839000000	0.611677000000	10.576970000000
C	-3.677737000000	3.062491000000	10.940830000000
C	-2.833722000000	3.361889000000	9.874417000000
C	-3.221813000000	4.279702000000	8.891776000000
C	-4.465535000000	4.900591000000	8.999469000000
C	-5.317073000000	4.594572000000	10.062484000000
C	-4.928415000000	3.675416000000	11.034550000000
C	-2.290983000000	4.525766000000	7.716505000000
C	-2.561942000000	5.750671000000	6.961795000000
C	-2.786811000000	6.766105000000	6.345104000000
H	-3.360375000000	2.348454000000	11.699702000000

H	-1.858030000000	2.879137000000	9.804096000000
H	-4.774209000000	5.614319000000	8.237215000000
H	-6.291394000000	5.076679000000	10.127912000000
H	-5.595323000000	3.435962000000	11.861460000000
H	-2.362411000000	3.672475000000	7.026059000000
H	-1.254784000000	4.558622000000	8.076835000000
H	-2.975766000000	7.667237000000	5.800915000000

Pr4F7

C	7.341915000000	0.884577000000	2.426382000000
C	6.272445000000	0.045431000000	2.718728000000
C	5.395175000000	0.417438000000	3.729446000000
C	5.543937000000	1.590970000000	4.455152000000
C	6.615097000000	2.424734000000	4.152173000000
C	7.521430000000	2.082321000000	3.137113000000
C	8.619965000000	2.952580000000	2.822028000000
C	9.543416000000	3.687109000000	2.551757000000
H	8.043261000000	0.622420000000	1.637312000000
H	6.100618000000	-0.876978000000	2.169541000000
H	4.810429000000	1.855296000000	5.214916000000
H	6.748641000000	3.357776000000	4.695517000000
H	10.361896000000	4.333944000000	2.315710000000
F	4.353530000000	-0.388541000000	4.007972000000
C	3.149897000000	4.625087000000	4.355176000000
C	3.735166000000	4.218522000000	3.160036000000
C	3.398274000000	2.989568000000	2.581517000000
C	2.450076000000	2.182918000000	3.207473000000
C	1.860717000000	2.588881000000	4.407272000000
C	2.210781000000	3.805727000000	4.987438000000
C	4.134204000000	2.566731000000	1.321843000000
C	3.722243000000	1.275134000000	0.771731000000
C	3.368814000000	0.206392000000	0.330561000000
H	3.425428000000	5.581836000000	4.796920000000
H	4.480691000000	4.851761000000	2.676983000000
H	2.188333000000	1.221965000000	2.768432000000
H	1.127103000000	1.945527000000	4.890952000000
H	1.752776000000	4.119795000000	5.924137000000
H	5.210407000000	2.522720000000	1.548302000000
H	4.007644000000	3.337780000000	0.550251000000
H	3.060806000000	-0.736098000000	-0.070205000000

Pr4F8

C	5.975522000000	2.466205000000	-0.590973000000
C	6.066901000000	3.737726000000	-0.031094000000
C	5.908294000000	3.869362000000	1.342169000000
C	5.657019000000	2.786856000000	2.173802000000
C	5.561641000000	1.522961000000	1.602161000000
C	5.724398000000	1.349147000000	0.218983000000
C	5.638462000000	0.038830000000	-0.362083000000
C	5.582535000000	-1.065877000000	-0.853615000000
H	6.097264000000	2.330792000000	-1.663465000000
H	6.259668000000	4.618591000000	-0.639383000000
H	5.502876000000	2.947064000000	3.239675000000
H	5.342336000000	0.658583000000	2.225305000000
H	5.534483000000	-2.041036000000	-1.289953000000
F	5.987330000000	5.100682000000	1.885673000000
C	3.004644000000	4.777923000000	4.036009000000
C	2.790995000000	4.397317000000	2.714546000000
C	2.532406000000	3.061856000000	2.388226000000
C	2.469337000000	2.115178000000	3.409504000000
C	2.680727000000	2.494574000000	4.737103000000
C	2.953917000000	3.823536000000	5.054577000000

C	2.378477000000	2.698100000000	0.921690000000
C	2.276894000000	1.264225000000	0.649629000000
C	2.215168000000	0.076969000000	0.431028000000
H	3.220950000000	5.818818000000	4.271799000000
H	2.855445000000	5.141782000000	1.919864000000
H	2.272715000000	1.073115000000	3.162339000000
H	2.633734000000	1.744896000000	5.525889000000
H	3.125509000000	4.116885000000	6.089063000000
H	3.247557000000	3.091128000000	0.373594000000
H	1.493627000000	3.203795000000	0.511718000000
H	2.171589000000	-0.969496000000	0.215756000000

Pr4F9

C	6.188287000000	1.680361000000	1.567757000000
C	6.334285000000	1.729838000000	0.184149000000
C	6.521676000000	2.965724000000	-0.416878000000
C	6.561696000000	4.151225000000	0.307464000000
C	6.416395000000	4.088841000000	1.689564000000
C	6.232594000000	2.854555000000	2.332296000000
C	6.078023000000	2.799048000000	3.758294000000
C	5.940942000000	2.755701000000	4.959630000000
H	6.021300000000	0.726954000000	2.064068000000
H	6.286021000000	0.832307000000	-0.427689000000
H	6.705985000000	5.095670000000	-0.212405000000
H	6.440975000000	4.999042000000	2.285153000000
H	5.807373000000	2.717509000000	6.019686000000
F	6.662615000000	3.023378000000	-1.756157000000
C	2.837328000000	4.625484000000	4.261075000000
C	2.986959000000	4.291302000000	2.919298000000
C	2.834295000000	2.967506000000	2.490611000000
C	2.536933000000	1.982467000000	3.430188000000
C	2.383684000000	2.316283000000	4.777932000000
C	2.529823000000	3.635535000000	5.197187000000
C	2.980449000000	2.673259000000	1.007103000000
C	2.958564000000	1.253524000000	0.653399000000
C	2.928797000000	0.077933000000	0.371354000000
H	2.960437000000	5.659591000000	4.579916000000
H	3.228995000000	5.065322000000	2.189476000000
H	2.424806000000	0.948984000000	3.106883000000
H	2.148893000000	1.536784000000	5.501576000000
H	2.409632000000	3.894773000000	6.248137000000
H	3.920084000000	3.113087000000	0.645448000000
H	2.170539000000	3.178555000000	0.462839000000
H	2.897371000000	-0.957674000000	0.106014000000

Pr4F10

C	2.313001000000	-2.573297000000	0.296287000000
C	2.848828000000	-2.709620000000	1.571569000000
C	2.440783000000	-1.824270000000	2.560928000000
C	1.510378000000	-0.822252000000	2.331679000000
C	0.978040000000	-0.699947000000	1.052511000000
C	1.378753000000	-1.563255000000	0.023785000000
C	0.852955000000	-1.394953000000	-1.302028000000
C	0.417061000000	-1.238053000000	-2.420657000000
H	2.623119000000	-3.242695000000	-0.503243000000
H	3.579065000000	-3.480757000000	1.806985000000
H	1.233162000000	-0.139703000000	3.133617000000
H	0.252724000000	0.083762000000	0.841439000000
H	0.028874000000	-1.107896000000	-3.408611000000
F	2.974986000000	-1.943655000000	3.793145000000
C	1.003848000000	2.913365000000	3.273067000000
C	1.409413000000	2.688306000000	1.958357000000

C	2.656850000000	2.121219000000	1.684429000000
C	3.501918000000	1.797661000000	2.747070000000
C	3.101793000000	2.026892000000	4.063379000000
C	1.850164000000	2.580325000000	4.331723000000
C	3.053424000000	1.861818000000	0.241024000000
C	4.022909000000	0.776406000000	0.078614000000
C	4.831680000000	-0.113333000000	-0.044798000000
H	0.024189000000	3.345652000000	3.471908000000
H	0.739945000000	2.939908000000	1.134675000000
H	4.465621000000	1.333697000000	2.542423000000
H	3.765648000000	1.757575000000	4.883443000000
H	1.533124000000	2.748020000000	5.359712000000
H	3.471428000000	2.779381000000	-0.196935000000
H	2.155462000000	1.615357000000	-0.341284000000
H	5.538529000000	-0.906665000000	-0.164285000000

Pr4F11

C	-0.089139000000	3.323030000000	-4.556053000000
C	-0.658083000000	3.054109000000	-5.796279000000
C	-1.040464000000	1.749221000000	-6.077853000000
C	-0.878147000000	0.710159000000	-5.173103000000
C	-0.307889000000	0.989723000000	-3.935663000000
C	0.092051000000	2.295707000000	-3.617024000000
C	0.668120000000	2.581800000000	-2.332513000000
C	1.127224000000	2.829622000000	-1.239987000000
H	0.221834000000	4.335247000000	-4.305623000000
H	-0.807199000000	3.833167000000	-6.540605000000
H	-1.201192000000	-0.294561000000	-5.436925000000
H	-0.182747000000	0.196028000000	-3.201481000000
H	1.514996000000	3.045194000000	-0.266991000000
C	-2.900736000000	-0.897502000000	-2.554978000000
C	-3.016712000000	0.402726000000	-2.068719000000
C	-2.156107000000	0.872337000000	-1.071585000000
C	-1.177194000000	0.016585000000	-0.564419000000
C	-1.056732000000	-1.285900000000	-1.051634000000
C	-1.916046000000	-1.747352000000	-2.048612000000
C	-2.292473000000	2.312912000000	-0.609756000000
C	-1.639956000000	2.610675000000	0.666161000000
C	-1.109091000000	2.843983000000	1.727267000000
H	-3.579573000000	-1.247707000000	-3.331337000000
H	-3.782138000000	1.065405000000	-2.473767000000
H	-0.505182000000	0.374892000000	0.213399000000
H	-0.288930000000	-1.943510000000	-0.646951000000
H	-1.824085000000	-2.765394000000	-2.423872000000
H	-3.357410000000	2.564073000000	-0.524282000000
H	-1.868108000000	2.973156000000	-1.380068000000
H	-0.653721000000	3.062093000000	2.670034000000
F	-1.594750000000	1.483728000000	-7.278075000000

Pr4F12

C	-3.215965000000	-0.698566000000	2.720295000000
C	-3.087626000000	0.686972000000	2.726845000000
C	-4.226011000000	1.457473000000	2.913130000000
C	-5.484008000000	0.901545000000	3.100547000000
C	-5.601761000000	-0.483522000000	3.086177000000
C	-4.473327000000	-1.293923000000	2.890538000000
C	-4.608032000000	-2.723203000000	2.851908000000
C	-4.727831000000	-3.927657000000	2.818838000000
H	-2.340687000000	-1.327030000000	2.564777000000
H	-2.122283000000	1.169825000000	2.588773000000
H	-6.344721000000	1.550528000000	3.245211000000
H	-6.574959000000	-0.950743000000	3.222639000000

H	-4.832540000000	-4.991681000000	2.799248000000
C	-0.108506000000	-1.636535000000	0.587016000000
C	-0.880824000000	-0.593266000000	0.078226000000
C	-2.206934000000	-0.810259000000	-0.305286000000
C	-2.747143000000	-2.091614000000	-0.185686000000
C	-1.975320000000	-3.138250000000	0.318081000000
C	-0.655824000000	-2.914523000000	0.709814000000
C	-3.027515000000	0.355539000000	-0.829552000000
C	-4.465715000000	0.223877000000	-0.585606000000
C	-5.649942000000	0.094264000000	-0.381201000000
H	0.919878000000	-1.450469000000	0.893341000000
H	-0.452862000000	0.406559000000	-0.004559000000
H	-3.790073000000	-2.262428000000	-0.448982000000
H	-2.416900000000	-4.127526000000	0.425306000000
H	-0.058036000000	-3.729076000000	1.115365000000
H	-2.859492000000	0.469155000000	-1.910015000000
H	-2.675947000000	1.281905000000	-0.357001000000
H	-6.698216000000	-0.010183000000	-0.198334000000
F	-4.105774000000	2.800739000000	2.913941000000

Pr4F13

C	3.041037000000	0.724162000000	3.055656000000
C	4.349963000000	0.261692000000	2.970264000000
C	4.732359000000	-0.430841000000	1.829282000000
C	3.862257000000	-0.676400000000	0.776629000000
C	2.556246000000	-0.207700000000	0.871626000000
C	2.134149000000	0.494343000000	2.010044000000
C	0.780863000000	0.966088000000	2.109346000000
C	-0.360339000000	1.360554000000	2.204057000000
H	2.711100000000	1.268749000000	3.937916000000
H	5.070565000000	0.427845000000	3.767939000000
H	4.207148000000	-1.227945000000	-0.095370000000
H	1.853165000000	-0.394714000000	0.062739000000
H	-1.380638000000	1.676544000000	2.274610000000
F	5.999723000000	-0.883394000000	1.742781000000
C	1.067526000000	-2.434475000000	-1.653475000000
C	0.120253000000	-1.411939000000	-1.698127000000
C	-0.672220000000	-1.124107000000	-0.582065000000
C	-0.506816000000	-1.879617000000	0.580242000000
C	0.442666000000	-2.900567000000	0.627707000000
C	1.232389000000	-3.181671000000	-0.486605000000
C	-1.644675000000	0.040265000000	-0.655558000000
C	-2.732928000000	-0.009249000000	0.322792000000
C	-3.630739000000	-0.056179000000	1.131442000000
H	1.673746000000	-2.649653000000	-2.532241000000
H	-0.005616000000	-0.830335000000	-2.611854000000
H	-1.117878000000	-1.658428000000	1.453507000000
H	0.567866000000	-3.476989000000	1.542818000000
H	1.972827000000	-3.978909000000	-0.446587000000
H	-2.079668000000	0.086067000000	-1.661878000000
H	-1.084900000000	0.975238000000	-0.505462000000
H	-4.433101000000	-0.098363000000	1.837506000000

Pr4F14

C	-3.060754000000	0.913118000000	3.383123000000
C	-4.429931000000	0.711256000000	3.514661000000
C	-5.035538000000	-0.240532000000	2.707478000000
C	-4.330621000000	-1.001967000000	1.786078000000
C	-2.962226000000	-0.790162000000	1.662144000000
C	-2.316272000000	0.169786000000	2.455301000000
C	-0.905360000000	0.392315000000	2.309452000000
C	0.279807000000	0.587940000000	2.159780000000

H	-2.556730000000	1.654505000000	3.999950000000
H	-5.029170000000	1.282791000000	4.219648000000
H	-4.855057000000	-1.736566000000	1.179126000000
H	-2.379396000000	-1.360897000000	0.942353000000
H	1.326677000000	0.753888000000	2.018727000000
C	0.709119000000	1.538611000000	-1.533349000000
C	-0.136207000000	2.361908000000	-0.796453000000
C	-1.474246000000	2.010323000000	-0.589230000000
C	-1.957194000000	0.828445000000	-1.147123000000
C	-1.109537000000	-0.002508000000	-1.883527000000
C	0.224754000000	0.345793000000	-2.075320000000
C	-2.331288000000	2.916871000000	0.276561000000
C	-3.748657000000	2.557451000000	0.332822000000
C	-4.917814000000	2.252051000000	0.371035000000
H	1.748746000000	1.825456000000	-1.686683000000
H	0.248168000000	3.286766000000	-0.364247000000
H	-3.001112000000	0.556135000000	-0.998653000000
H	-1.497942000000	-0.925390000000	-2.312767000000
H	0.884481000000	-0.302239000000	-2.650265000000
H	-2.241667000000	3.950533000000	-0.082715000000
H	-1.924302000000	2.902113000000	1.298813000000
H	-5.953611000000	1.988901000000	0.418621000000
F	-6.367553000000	-0.426942000000	2.815222000000