

## Supporting information

# Rational Design of Porous Organic Molecules Based on B-Heterocyclic Carbenes

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Table 1S The number of imaginary frequency ( $N_{\text{imag}}$ ), energy including zero point energy ( $E$ , in Hartree) and relative energy ( $E_{\text{R}}$ , in kcal·mol<sup>-1</sup>) of the blocks at M06-2X/6-311+G\*\* and B3LYP/6-31G\*\* levels.

Motifs	$N_{\text{imag}}^{\text{a)}$	$E^{\text{a)}$	$E_{\text{R}}^{\text{a)}$	$N_{\text{imag}}^{\text{b)}$	$E^{\text{b)}$	$E_{\text{R}}^{\text{b)}$
<b>B1-p</b>	0	-445.38828	0.0	0	-445.45518	0.0
<b>B1-c</b>	3	-445.37266	9.8	3	-445.44046	9.2
<b>B2-p</b>	0	-673.88129	0.0	0	-673.98508	0.0
<b>B2-c</b>	3	-673.87592	3.4	3	-673.97991	3.2
<b>B3-p</b>	0	-902.28758	0.0	0	-902.43311	0.0
<b>B3-c</b>	3	-902.28506	1.6	3	-902.43021	1.8
<b>B4-p</b>	0	-305.77912	0.0	0	-305.83139	0.0
<b>B4-c</b>	2	-305.76918	6.2	2	-305.82253	5.6
<b>B5-p</b>	0	-458.11218	0.0	0	-458.18976	0.0
<b>B5-c</b>	2	-458.10814	2.5	2	-458.18538	2.7
<b>B6-p</b>	0	-610.38293	0.0	0	-610.48844	0.0
<b>B6-c</b>	2	-610.38111	1.1	2	-610.48602	1.5

a) M06-2X/6-311+G\*\*, b) B3LYP/6-31G\*\*

Table 2S First vertical transition energies ( $\lambda$ , in nm) and oscillator strengths ( $f$ ) of POM-n (n=1-36).

n	transition	$\lambda$	$f$	n	transition	$\lambda$	$f$
1	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>1u</sub>	325.03	0.1113	19	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>1u</sub>	319.31	0.0088
2	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	341.73	0.0243	20	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	339.19	0.0351
3	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>u</sub>	338.45	0.1806	21	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> A <sub>u</sub>	337.56	0.0023
4	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	348.69	0.0014	22	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	348.40	0.0009
5	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>u</sub>	346.53	0.0306	23	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>u</sub>	345.96	0.0309
6	<sup>1</sup> A <sub>1</sub> '→ <sup>1</sup> E'	353.18	0.1157	24	<sup>1</sup> A <sub>1</sub> '→ <sup>1</sup> E'	351.40	0.1179
7	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>3u</sub>	368.06	0.5133	25	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>2u</sub>	349.67	0.2730
8	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	398.33	0.0668	26	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	396.36	0.0858
9	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>u</sub>	396.02	0.2142	27	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>u</sub>	394.50	0.2768
10	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	402.70	0.0043	28	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	402.42	0.0020
11	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>u</sub>	401.23	0.0493	29	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>u</sub>	400.63	0.0420
12	<sup>1</sup> A <sub>1</sub> '→ <sup>1</sup> E'	409.89	0.2282	30	<sup>1</sup> A <sub>1</sub> '→ <sup>1</sup> E'	408.81	0.2190
13	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>3u</sub>	441.00	0.6497	31	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>3u</sub>	413.47	0.3891
14	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	470.82	0.1136	32	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	468.78	0.1546
15	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>u</sub>	469.86	0.3237	33	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>u</sub>	467.24	0.4303
16	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	473.94	0.0098	34	<sup>1</sup> A <sub>1</sub> → <sup>1</sup> A <sub>1</sub>	473.58	0.0044
17	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>u</sub>	472.70	0.0774	35	<sup>1</sup> A <sub>g</sub> → <sup>1</sup> B <sub>u</sub>	471.99	0.0611
18	<sup>1</sup> A <sub>1</sub> '→ <sup>1</sup> E'	487.86	0.3256	36	<sup>1</sup> A <sub>1</sub> '→ <sup>1</sup> E'	481.60	0.3212

Table 3S The length (in angstrom) and WBIs of Ag-C( $\equiv$ C), ptC-Ag, ptC-B, ptC-C(CH) and ptC-C bonds **C1-C3** and MOF-BHC-1.

Species	Ag-C( $\equiv$ C)	ptC-Ag	ptC-B	ptC-C(CH)	ptC-C
	Bond length				
<b>C1</b>	2.01	2.11	1.52	1.54	1.47
<b>C2</b>	2.01	2.11	1.52	1.54	1.47
<b>C3</b>	2.01	2.11	1.52	1.54	1.47
MOF-BHC-1	1.95	2.00, 2.01	1.53	1.50, .53	1.45, 1.46
	WBIs				
<b>C1</b>	0.73	0.31	0.94	0.87	1.26
<b>C2</b>	0.73	0.31	0.94	0.87	1.26
<b>C3</b>	0.73	0.31	0.94	0.87	1.26

**Cartesian coordinates, electronic energy (E) and the smallest vibrational frequency ( $\nu$ ) for all the stable molecules calculated at the B3LYP/6-31G\*\* level, as well as cartesian coordinates and electronic energy (E) for COFs and MOF calculated at the RLSDA level.**

**B1-p**

E= -445.5803624  
 $\nu$ = 43.2490

B	0.000000	0.000000	0.000000
B	0.000000	1.660687	0.000000
B	1.438197	-0.830344	0.000000
B	-1.438197	-0.830344	0.000000
C	0.000000	2.930276	0.730230
C	0.000000	2.930276	-0.730230
C	2.537693	-1.465138	0.730230
C	2.537693	-1.465138	-0.730230
C	-2.537693	-1.465138	0.730230
C	-2.537693	-1.465138	-0.730230
C	3.647307	-2.105774	0.000000
H	4.622897	-1.617944	0.000000
H	3.712629	-3.194574	0.000000
C	0.000000	4.211547	0.000000
H	0.910268	4.812518	0.000000
H	-0.910268	4.812518	0.000000
C	-3.647307	-2.105774	0.000000
H	-4.622897	-1.617944	0.000000
H	-3.712629	-3.194574	0.000000

**B2-p**

E= -674.141038901  
 $\nu$ = 20.1920

B	3.665846	-2.116477	0.000000
B	-3.665846	-2.116477	0.000000
B	0.000000	4.232954	0.000000
C	-5.859452	-3.382956	0.000000
H	-5.924528	-4.471732	0.000000
C	5.859452	-3.382956	0.000000
H	6.834897	-2.894926	0.000000
H	5.924528	-4.471732	0.000000
C	0.000000	6.765913	0.000000
H	0.910370	7.366658	0.000000
B	0.000000	0.000000	0.000000
C	0.000000	1.515822	0.000000
C	0.000000	2.740170	0.000000
C	-1.312740	-0.757911	0.000000
C	-2.373057	-1.370085	0.000000
C	1.312740	-0.757911	0.000000
C	2.373057	-1.370085	0.000000
C	0.000000	5.490183	0.737475
C	0.000000	5.490183	-0.737475
C	4.754638	-2.745092	0.737475
C	4.754638	-2.745092	-0.737475
C	-4.754638	-2.745092	0.737475
C	-4.754638	-2.745092	-0.737475
H	-6.834897	-2.894926	0.000000
H	-0.910370	7.366658	0.000000

**B3-p**

E= -902.620828951  
 $\nu$ = 11.5592

B	5.897290	-3.404802	0.000000
B	-5.897290	-3.404802	0.000000
B	0.000000	6.809604	0.000000
C	-8.090980	-4.671330	0.000000

H	-8.155415	-5.759987	0.000000
C	8.090980	-4.671330	0.000000
H	9.066003	-4.182803	0.000000
H	8.155415	-5.759987	0.000000
C	0.000000	9.342659	0.000000
H	0.910588	9.942790	0.000000
B	0.000000	0.000000	0.000000
C	0.000000	1.512200	0.000000
C	-1.309604	-0.756100	0.000000
C	1.309604	-0.756100	0.000000
C	0.000000	8.067148	0.737726
C	0.000000	8.067148	-0.737726
C	6.986355	-4.033574	0.737726
C	6.986355	-4.033574	-0.737726
C	-6.986355	-4.033574	0.737726
C	-6.986355	-4.033574	-0.737726
H	-9.066003	-4.182803	0.000000
H	-0.910588	9.942790	0.000000
C	0.000000	2.740024	0.000000
C	0.000000	4.095100	0.000000
C	-2.372930	-1.370012	0.000000
C	-3.546461	-2.047550	0.000000
C	-4.607360	-2.660060	0.000000
C	2.372930	-1.370012	0.000000
C	3.546461	-2.047550	0.000000
C	4.607360	-2.660060	0.000000
C	0.000000	5.320121	0.000000

**B4-p**

E= -305.9241371  
 $\nu$ = 50.6904

B	0.000000	0.000000	1.312708
B	0.000000	1.462306	0.523265
B	0.000000	-1.462306	0.523265
C	0.730550	2.577211	-0.084868
C	-0.730550	2.577211	-0.084868
C	0.730550	-2.577211	-0.084868
C	-0.730550	-2.577211	-0.084868
C	0.000000	-3.703429	-0.695274
H	0.000000	-3.797900	-1.781744
H	0.000000	-4.665345	-0.181415
C	0.000000	3.703429	-0.695274
H	0.000000	3.797900	-1.781744
H	0.000000	4.665345	-0.181415
H	0.000000	0.000000	2.510263

**B5-p**

E= -458.303480955  
 $\nu$ = 23.2523

B	0.000000	-3.714009	-0.033243
B	0.000000	3.714009	-0.033243
C	0.000000	-5.950299	-1.223931
H	0.000000	-6.052933	-2.309668
H	0.000000	-6.908463	-0.703082
C	0.000000	5.950299	-1.223931
H	0.000000	6.052933	-2.309668
B	0.000000	0.000000	1.979242
C	0.000000	1.315554	1.244129
C	0.000000	2.397801	0.668952

C	0.000000	-1.315554	1.244129
C	0.000000	-2.397801	0.668952
C	0.737038	4.824117	-0.624225
C	-0.737038	4.824117	-0.624225
C	0.737038	-4.824117	-0.624225
C	-0.737038	-4.824117	-0.624225
H	0.000000	6.908463	-0.703082
H	0.000000	0.000000	3.173342

**B6-p**

E= -610.623390720

v= 13.2586

B	0.000000	5.980442	-0.606112
B	0.000000	-5.980442	-0.606112
C	0.000000	-8.214217	-1.799457
H	0.000000	-8.315597	-2.885341
C	0.000000	8.214217	-1.799457
H	0.000000	9.173138	-1.279941
H	0.000000	8.315597	-2.885341
B	0.000000	0.000000	2.631165
C	0.000000	-1.310274	1.895159
C	0.000000	1.310274	1.895159
C	0.738047	7.089451	-1.198662
C	-0.738047	7.089451	-1.198662
C	0.738047	-7.089451	-1.198662
C	-0.738047	-7.089451	-1.198662
H	0.000000	-9.173138	-1.279941
C	0.000000	-2.393737	1.314718
C	0.000000	-3.587292	0.674773
C	0.000000	-4.667374	0.096306
C	0.000000	2.393737	1.314718
C	0.000000	3.587292	0.674773
C	0.000000	4.667374	0.096306
H	0.000000	0.0000 800	3.825751

**POM-1**

E= -1041.04250763

v= 15.3774

B	-4.327802	0.000000	0.000000
B	-3.463710	1.417158	0.000000
B	-5.986824	0.000000	0.000000
B	-3.463710	-1.417158	0.000000
C	-8.536220	0.000000	0.000000
H	-9.136616	0.910265	0.000000
H	-9.136616	-0.910265	0.000000
C	-2.052468	3.556534	0.000000
H	-2.503459	4.550893	0.000000
C	-2.052468	-3.556534	0.000000
H	-2.503459	-4.550893	0.000000
B	4.327802	0.000000	0.000000
B	3.463710	1.417158	0.000000
B	3.463710	-1.417158	0.000000
B	5.986824	0.000000	0.000000
C	2.052468	-3.556534	0.000000
H	2.503459	-4.550893	0.000000
C	2.052468	3.556534	0.000000
H	2.503459	4.550893	0.000000
C	8.536220	0.000000	0.000000
H	9.136616	0.910265	0.000000
H	9.136616	-0.910265	0.000000
C	-0.604853	3.574458	0.000000
C	0.604853	3.574458	0.000000
C	-0.604853	-3.574458	0.000000
C	0.604853	-3.574458	0.000000
C	-2.781233	-2.489183	0.729459
C	-2.781233	-2.489183	-0.729459
C	2.781233	-2.489183	0.729459
C	2.781233	-2.489183	-0.729459
C	2.781233	2.489183	0.729459

C	2.781233	2.489183	-0.729459
C	-2.781233	2.489183	0.729459
C	-2.781233	2.489183	-0.729459
C	-7.255134	0.000000	0.730637
C	-7.255134	0.000000	-0.730637
C	7.255134	0.000000	0.730637
C	7.255134	0.000000	-0.730637

**POM-2**

E= -1636.50045157

v= 9.6977

B	0.000000	0.000000	-2.909626
B	0.000000	0.000000	-1.250236
B	0.000000	1.461449	-3.691758
B	0.000000	-1.461449	-3.691758
C	0.000000	3.776985	-4.788095
H	0.000000	3.910510	-5.871614
C	0.000000	0.000000	1.324163
C	0.000000	-3.776985	-4.788095
H	0.000000	-3.910510	-5.871614
B	0.000000	-7.305091	1.601363
B	0.000000	-5.827534	2.357971
B	0.000000	-7.319969	-0.058428
C	0.000000	-8.716442	2.473779
B	0.000000	-3.512926	3.458266
H	0.000000	-3.383771	4.542423
C	0.000000	-10.884778	3.814156
H	0.000000	-10.916970	4.904115
C	0.000000	-1.226652	2.104657
C	0.000000	-2.263649	2.726309
C	0.000000	-5.019571	-4.045407
C	0.000000	-6.045638	-3.404662
B	0.000000	7.305091	1.601363
B	0.000000	8.716442	2.473779
B	0.000000	5.827534	2.357971
B	0.000000	7.319969	-0.058428
C	0.000000	3.512926	3.458266
H	0.000000	3.383771	4.542423
C	0.000000	10.884778	3.814156
H	0.000000	10.916970	4.904115
H	0.000000	11.874126	3.355569
C	0.000000	7.262763	-2.620732
H	0.000000	8.173237	-3.223287
C	0.000000	6.045638	-3.404662
C	0.000000	2.263649	2.726309
C	0.000000	1.226652	2.104657
C	0.000000	5.019571	-4.045407
C	0.730623	9.795125	3.140591
C	-0.730623	9.795125	3.140591
C	-0.729461	7.312496	-1.329242
C	0.729461	7.312496	-1.329242
C	-0.729726	2.599153	-4.255937
C	0.729726	2.599153	-4.255937
C	-0.729395	4.687749	2.920604
C	0.729395	4.687749	2.920604
C	-0.729383	0.000000	0.021031
C	0.729383	0.000000	0.021031
C	-0.729395	-4.687749	2.920604
C	0.729395	-4.687749	2.920604
C	0.729726	-2.599153	-4.255937
C	-0.729726	-2.599153	-4.255937
C	0.729461	-7.312496	-1.329242
C	-0.729461	-7.312496	-1.329242
C	-0.730623	-9.795125	3.140591
C	0.730623	-9.795125	3.140591
H	0.000000	-11.874126	3.355569
C	0.000000	-7.262763	-2.620732
H	0.000000	-8.173237	-3.223287

**POM-3**

E= -2231.95834981

v= 4.7579

B	-2.638232	3.344956	0.000000
B	-0.990580	3.540954	0.000000
B	-3.588622	4.703307	0.000000
B	-3.252436	1.804982	0.000000
C	-4.956661	6.869261	0.000000
H	-6.048357	6.871430	0.000000
C	1.565253	3.850906	0.000000
C	-4.097470	-0.613429	0.000000
H	-5.160429	-0.862286	0.000000
B	2.638232	-3.344956	0.000000
B	3.252436	-1.804982	0.000000
B	0.990580	-3.540954	0.000000
B	3.588622	-4.703307	0.000000
C	-1.565253	-3.850906	0.000000
C	4.097470	0.613429	0.000000
H	5.160429	0.862286	0.000000
C	4.956661	-6.869261	0.000000
H	6.048357	-6.871430	0.000000
C	2.487442	2.726795	0.000000
C	3.228179	1.771233	0.000000
C	-3.228179	-1.771233	0.000000
C	-2.487442	-2.726795	0.000000
B	-0.964148	-11.135069	0.000000
B	0.685486	-10.951496	0.000000
B	-1.660064	-12.641374	0.000000
B	-1.893260	-9.759491	0.000000
C	-2.727623	-14.956100	0.000000
H	-2.152648	-15.882656	0.000000
H	-3.805654	-15.120281	0.000000
C	3.222750	-10.589613	0.000000
H	3.929483	-11.421838	0.000000
C	-3.263719	-7.593868	0.000000
H	-4.355534	-7.594872	0.000000
C	-2.192962	-5.162168	0.000000
C	4.368539	-8.191932	0.000000
C	3.856005	-9.287685	0.000000
C	-2.685893	-6.266177	0.000000
C	-2.191106	-13.792876	0.730684
C	-2.191106	-13.792876	-0.730684
B	0.964148	11.135069	0.000000
B	1.660064	12.641374	0.000000
B	1.893260	9.759491	0.000000
B	-0.685486	10.951496	0.000000
C	3.263719	7.593868	0.000000
H	4.355534	7.594872	0.000000
C	2.727623	14.956100	0.000000
H	3.805654	15.120281	0.000000
H	2.152648	15.882656	0.000000
C	-3.222750	10.589613	0.000000
H	-3.929483	11.421838	0.000000
C	-3.856005	9.287685	0.000000
C	2.685893	6.266177	0.000000
C	2.192962	5.162168	0.000000
C	-4.368539	8.191932	0.000000
C	2.191106	13.792876	-0.730684
C	2.191106	13.792876	0.730684
C	-1.946343	10.792457	0.729464
C	-1.946343	10.792457	-0.729464
C	-4.286801	5.763849	0.729778
C	-4.286801	5.763849	-0.729778
C	2.589473	8.695947	0.729385
C	2.589473	8.695947	-0.729385
C	0.271551	3.693631	0.729326
C	0.271551	3.693631	-0.729326
C	3.692302	-0.613409	0.729688
C	3.692302	-0.613409	-0.729688

C	-3.692302	0.613409	-0.729688
C	-3.692302	0.613409	0.729688
C	-2.589473	-8.695947	0.729385
C	-2.589473	-8.695947	-0.729385
C	-0.271551	-3.693631	-0.729326
C	-0.271551	-3.693631	0.729326
C	4.286801	-5.763849	0.729778
C	4.286801	-5.763849	-0.729778
C	1.946343	-10.792457	0.729464
C	1.946343	-10.792457	-0.729464

**POM-4**

E= -2827.41622465

v= 3.5052

B	0.000000	7.273886	2.622740
B	0.000000	7.271962	0.963439
B	0.000000	8.736709	3.402749
B	0.000000	5.818045	3.415945
C	0.000000	11.052131	4.498854
H	0.000000	11.185502	5.582395
C	0.000000	7.275306	-1.611069
C	0.000000	3.517624	4.543420
H	0.000000	3.397763	5.628522
B	0.000000	0.000000	-1.816355
B	0.000000	1.457237	-2.607388
B	0.000000	0.000000	-0.157042
B	0.000000	-1.457237	-2.607388
C	0.000000	0.000000	2.417583
C	0.000000	3.757023	-3.735778
H	0.000000	3.875906	-4.820980
C	0.000000	-3.757023	-3.735778
H	0.000000	-3.875906	-4.820980
C	0.000000	6.048708	-2.391854
C	0.000000	5.011072	-3.012402
C	0.000000	2.263936	3.819150
C	0.000000	1.226714	3.197904
B	0.000000	-7.273886	2.622740
B	0.000000	-7.271962	0.963439
B	0.000000	-8.736709	3.402749
B	0.000000	-5.818045	3.415945
C	0.000000	-11.052131	4.498854
H	0.000000	-11.185502	5.582395
C	0.000000	-7.275306	-1.611069
C	0.000000	-3.517624	4.543420
H	0.000000	-3.397763	5.628522
C	0.000000	-1.226714	3.197904
C	0.000000	-5.011072	-3.012402
C	0.000000	-6.048708	-2.391854
C	0.000000	-2.263936	3.819150
C	0.729793	-9.874163	3.966890
C	-0.729793	-9.874163	3.966890
B	0.000000	14.580506	-1.889471
B	0.000000	15.991381	-2.762719
B	0.000000	13.102853	-2.645914
B	0.000000	14.596038	-0.229728
C	0.000000	10.787918	-3.745517
H	0.000000	10.658069	-4.829599
C	0.000000	18.158748	-4.104453
H	0.000000	18.190458	-5.194441
H	0.000000	19.148384	-3.646504
C	0.000000	14.538482	2.332560
H	0.000000	15.448730	2.935461
C	0.000000	13.320935	3.115901
C	0.000000	9.538945	-3.012907
C	0.000000	8.502154	-2.390921
C	0.000000	12.294620	3.756241
C	-0.730671	17.069462	-3.430323
C	0.730671	17.069462	-3.430323
C	0.729469	14.588440	1.041105

C	-0.729469	14.588440	1.041105
C	0.729793	9.874163	3.966890
C	-0.729793	9.874163	3.966890
C	0.729383	11.962838	-3.208256
C	-0.729383	11.962838	-3.208256
C	0.729353	7.273494	-0.307867
C	-0.729353	7.273494	-0.307867
C	0.729698	2.587716	-3.186072
C	-0.729698	2.587716	-3.186072
C	-0.729631	4.687095	3.994267
C	0.729631	4.687095	3.994267
C	-0.729631	-4.687095	3.994267
C	-0.729335	0.000000	1.114321
C	0.729335	0.000000	1.114321
C	0.729698	-2.587716	-3.186072
C	-0.729698	-2.587716	-3.186072
C	0.729353	-7.273494	-0.307867
C	-0.729353	-7.273494	-0.307867
B	0.000000	-14.580506	-1.889471
B	0.000000	-13.102853	-2.645914
B	0.000000	-14.596038	-0.229728
B	0.000000	-15.991381	-2.762719
C	0.000000	-14.538482	2.332560
C	0.000000	-10.787918	-3.745517
H	0.000000	-10.658069	-4.829599
C	0.000000	-18.158748	-4.104453
H	0.000000	-18.190458	-5.194441
C	0.000000	-8.502154	-2.390921
C	0.000000	-9.538945	-3.012907
C	0.000000	-12.294620	3.756241
C	0.000000	-13.320935	3.115901
C	0.729383	-11.962838	-3.208256
C	-0.729383	-11.962838	-3.208256
C	-0.729469	-14.588440	1.041105
C	0.729469	-14.588440	1.041105
C	0.730671	-17.069462	-3.430323
C	-0.730671	-17.069462	-3.430323
H	0.000000	-15.448730	2.935461
H	0.000000	-19.148384	-3.646504

**POM-5**

E= -3422.87410206

v= 2.2375

B	-2.041467	3.741324	0.000000
B	-0.384132	3.660951	0.000000
B	-2.759759	5.235709	0.000000
B	-2.901519	2.323771	0.000000
C	-3.771644	7.589008	0.000000
H	-4.849543	7.762005	0.000000
C	2.187437	3.536622	0.000000
C	-4.138779	0.080651	0.000000
H	-5.228414	0.013738	0.000000
B	2.041467	-3.741324	0.000000
B	2.901519	-2.323771	0.000000
B	0.384132	-3.660951	0.000000
B	2.759759	-5.235709	0.000000
C	-2.187437	-3.536622	0.000000
C	4.138779	-0.080651	0.000000
H	5.228414	-0.013738	0.000000
C	3.771644	-7.589008	0.000000
H	4.849543	-7.762005	0.000000
C	2.906971	2.273260	0.000000
C	3.476385	1.206723	0.000000
C	-3.476385	-1.206723	0.000000
C	-2.906971	-2.273260	0.000000
B	-2.753205	-10.791829	0.000000
B	-1.095803	-10.870642	0.000000
B	-3.603999	-12.214598	0.000000
B	-3.473427	-9.298528	0.000000

C	-4.813106	-14.473090	0.000000
H	-5.901888	-14.552912	0.000000
C	1.475555	-10.997961	0.000000
C	-4.484734	-6.944759	0.000000
H	-5.562492	-6.770838	0.000000
C	-3.027011	-4.723534	0.000000
C	2.986560	-8.805380	0.000000
C	2.315396	-9.811003	0.000000
C	-3.698856	-5.728703	0.000000
C	-4.223702	-13.322752	0.729790
C	-4.223702	-13.322752	-0.729790
B	2.753205	10.791829	0.000000
B	3.603999	12.214598	0.000000
B	3.473427	9.298528	0.000000
B	1.095803	10.870642	0.000000
C	4.484734	6.944759	0.000000
H	5.562492	6.770838	0.000000
C	4.813106	14.473090	0.000000
H	5.901888	14.552912	0.000000
C	-1.475555	10.997961	0.000000
C	-2.315396	9.811003	0.000000
C	3.698856	5.728703	0.000000
C	3.027011	4.723534	0.000000
C	-2.986560	8.805380	0.000000
C	4.223702	13.322752	-0.729790
C	4.223702	13.322752	0.729790
C	-0.173994	10.932884	0.729349
C	-0.173994	10.932884	-0.729349
C	-3.281071	6.393699	0.729724
C	-3.281071	6.393699	-0.729724
C	3.994542	8.140101	0.729643
C	3.994542	8.140101	-0.729643
C	0.885751	3.599896	0.729336
C	0.885751	3.599896	-0.729336
C	3.533641	-1.222217	0.729668
C	3.533641	-1.222217	-0.729668
C	-3.533641	1.222217	-0.729668
C	-3.533641	1.222217	0.729668
C	-3.994542	-8.140101	0.729643
C	-3.994542	-8.140101	-0.729643
C	-0.885751	-3.599896	-0.729336
C	-0.885751	-3.599896	0.729336
C	3.281071	-6.393699	0.729724
C	3.281071	-6.393699	-0.729724
C	0.173994	-10.932884	0.729349
C	0.173994	-10.932884	-0.729349
B	1.395842	-18.307346	0.000000
B	2.224024	-16.868763	0.000000
B	-0.262663	-18.241711	0.000000
B	2.197716	-19.759975	0.000000
C	-2.819213	-18.060794	0.000000
C	3.435971	-14.610576	0.000000
H	4.525100	-14.533955	0.000000
C	3.428759	-21.992103	0.000000
H	4.515779	-22.078454	0.000000
C	2.194865	-12.261253	0.000000
C	2.765324	-13.327258	0.000000
C	-4.132473	-15.750584	0.000000
C	-3.543034	-16.806946	0.000000
C	2.841792	-15.757786	0.729365
C	2.841792	-15.757786	-0.729365
C	-1.531647	-18.172758	-0.729461
C	-1.531647	-18.172758	0.729461
C	2.810181	-20.870304	0.730656
C	2.810181	-20.870304	-0.730656
H	-3.465222	-18.940973	0.000000
H	2.921641	-22.957458	0.000000
B	-1.395842	18.307346	0.000000
B	0.262663	18.241711	0.000000

B	-2.224024	16.868763	0.000000
B	-2.197716	19.759975	0.000000
C	-3.435971	14.610576	0.000000
H	-4.525100	14.533955	0.000000
C	-2.841792	15.757786	0.729365
C	-2.841792	15.757786	-0.729365
C	-2.810181	20.870304	0.730656
C	-2.810181	20.870304	-0.730656
C	1.531647	18.172758	0.729461
C	1.531647	18.172758	-0.729461
C	3.543034	16.806946	0.000000
C	4.132473	15.750584	0.000000
C	-2.765324	13.327258	0.000000
C	-2.194865	12.261253	0.000000
C	-3.428759	21.992103	0.000000
H	-2.921641	22.957458	0.000000
H	-4.515779	22.078454	0.000000
C	2.819213	18.060794	0.000000
H	3.465222	18.940973	0.000000

**POM-6**

E= -2231.95382190

v= 8.4481

B	0.000000	0.000000	0.000000
B	0.000000	1.655407	0.000000
B	1.433624	-0.827703	0.000000
B	-1.433624	-0.827703	0.000000
C	3.661959	-2.114233	0.000000
C	0.000000	4.228467	0.000000
C	-3.661959	-2.114233	0.000000
B	-7.277034	4.201398	0.000000
B	-5.831515	5.018337	0.000000
B	-7.261765	2.541072	0.000000
B	-8.714635	5.031397	0.000000
C	-3.580067	6.243934	0.000000
H	-3.508880	7.333333	0.000000
C	-10.922105	6.305880	0.000000
H	-10.986997	7.394379	0.000000
C	-1.233405	4.997817	0.000000
C	-2.295311	5.576018	0.000000
C	-4.944939	-1.430749	0.000000
C	-5.976629	-0.800211	0.000000
B	7.277034	4.201398	0.000000
B	8.714635	5.031397	0.000000
B	5.831515	5.018337	0.000000
B	7.261765	2.541072	0.000000
C	3.580067	6.243934	0.000000
H	3.508880	7.333333	0.000000
C	10.922105	6.305880	0.000000
H	10.986997	7.394379	0.000000
H	11.897218	5.817829	0.000000
C	7.197439	-0.021538	0.000000
H	8.105293	-0.627887	0.000000
C	5.976629	-0.800211	0.000000
C	2.295311	5.576018	0.000000
C	1.233405	4.997817	0.000000
C	4.944939	-1.430749	0.000000
C	9.812706	5.665368	0.730669
C	9.812706	5.665368	-0.730669
C	7.249907	1.269746	-0.729317
C	7.249907	1.269746	0.729317
C	2.533506	-1.462720	-0.729713
C	2.533506	-1.462720	0.729713
C	4.724586	5.643731	-0.729317
C	4.724586	5.643731	0.729317
C	0.000000	2.925440	-0.729713
C	0.000000	2.925440	0.729713
C	-4.724586	5.643731	-0.729317
C	-4.724586	5.643731	0.729317
C	-2.533506	-1.462720	0.729713

C	-2.533506	-1.462720	-0.729713
C	-7.249907	1.269746	0.729317
C	-7.249907	1.269746	-0.729317
C	-9.812706	5.665368	-0.730669
C	-9.812706	5.665368	0.730669
H	-11.897218	5.817829	0.000000
C	-7.197439	-0.021538	0.000000
H	-8.105293	-0.627887	0.000000
B	0.000000	-8.402795	0.000000
B	1.430250	-7.559409	0.000000
B	-1.430250	-7.559409	0.000000
B	0.000000	-10.062794	0.000000
C	-3.617372	-6.222396	0.000000
C	3.617372	-6.222396	0.000000
H	4.596413	-6.705446	0.000000
C	0.000000	-12.611760	0.000000
H	0.910221	-13.212208	0.000000
C	2.525321	-6.913477	0.729317
C	2.525321	-6.913477	-0.729317
C	0.000000	-11.330737	-0.730669
C	0.000000	-11.330737	0.730669
C	-2.525321	-6.913477	-0.729317
C	-2.525321	-6.913477	0.729317
C	3.681318	-4.775807	0.000000
C	3.711534	-3.567069	0.000000
C	-3.681318	-4.775807	0.000000
C	-3.711534	-3.567069	0.000000
H	-0.910221	-13.212208	0.000000
H	-4.596413	-6.705446	0.000000

**POM-7**

E= -1650.47469226

v= 5.2177

B	-11.214782	0.000000	0.000000
B	-4.758758	3.597953	0.000000
B	-4.758758	-3.597953	0.000000
C	-3.342030	5.715238	0.000000
H	-3.789705	6.711727	0.000000
C	-13.747028	0.000000	0.000000
H	-14.347599	-0.910290	0.000000
H	-14.347599	0.910290	0.000000
C	-3.342030	-5.715238	0.000000
H	-3.789705	-6.711727	0.000000
B	-6.983310	0.000000	0.000000
C	-6.214055	-1.307018	0.000000
C	-5.571395	-2.349152	0.000000
C	-6.214055	1.307018	0.000000
C	-5.571395	2.349152	0.000000
C	-8.497201	0.000000	0.000000
C	-9.721531	0.000000	0.000000
C	-1.897475	-5.731044	0.000000
C	-0.681380	-5.742291	0.000000
C	0.681380	-5.742291	0.000000
C	1.897475	-5.731044	0.000000
C	-4.074363	-4.655390	0.736083
C	-4.074363	-4.655390	-0.736083
C	-12.471439	0.000000	0.737662
C	-12.471439	0.000000	-0.737662
C	-4.074363	4.655390	0.736083
C	-4.074363	4.655390	-0.736083
B	11.214782	0.000000	0.000000
B	4.758758	-3.597953	0.000000
B	4.758758	3.597953	0.000000
C	3.342030	-5.715238	0.000000
H	3.789705	-6.711727	0.000000
C	13.747028	0.000000	0.000000
H	14.347599	0.910290	0.000000
H	14.347599	-0.910290	0.000000
C	3.342030	5.715238	0.000000



H	3.789705	6.711727	0.000000
B	6.983310	0.000000	0.000000
C	6.214055	1.307018	0.000000
C	5.571395	2.349152	0.000000
C	6.214055	-1.307018	0.000000
C	5.571395	-2.349152	0.000000
C	8.497201	0.000000	0.000000
C	9.721531	0.000000	0.000000
C	1.897475	5.731044	0.000000
C	0.681380	5.742291	0.000000
C	-0.681380	5.742291	0.000000
C	-1.897475	5.731044	0.000000
C	4.074363	4.655390	0.736083
C	4.074363	4.655390	-0.736083
C	12.471439	0.000000	0.737662
C	12.471439	0.000000	-0.737662
C	4.074363	-4.655390	0.736083
C	4.074363	-4.655390	-0.736083

**POM-8**

E= -2626.80396634

v= 3.3009

B	0.000000	8.021664	-4.570835
B	0.000000	11.801647	1.573275
B	0.000000	15.397593	-4.875438
C	0.000000	11.727456	4.119682
C	0.000000	5.716004	-5.654246
H	0.000000	5.585116	-6.738783
C	0.000000	17.553813	-6.202921
H	0.000000	17.588172	-7.292880
B	0.000000	11.794381	-2.657026
C	0.000000	13.083369	-3.450618
C	0.000000	14.125943	-4.092536
C	0.000000	11.825076	-1.140661
C	0.000000	11.828984	0.083698
C	0.000000	10.454353	-3.367942
C	0.000000	9.363256	-3.923392
C	0.737697	16.467618	-5.534202
C	-0.737697	16.467618	-5.534202
C	0.736026	6.889473	-5.123643
C	-0.736026	6.889473	-5.123643
C	0.736122	11.784399	2.832866
C	-0.736122	11.784399	2.832866
B	0.000000	3.742883	6.577252
B	0.000000	0.000000	0.381536
B	0.000000	-3.742883	6.577252
C	0.000000	0.000000	-2.178956
C	0.000000	6.052363	7.650810
H	0.000000	6.189517	8.734483
C	0.000000	-6.052363	7.650810
H	0.000000	-6.189517	8.734483
B	0.000000	0.000000	4.610382
C	0.000000	-1.320068	5.353511
C	0.000000	-2.403234	5.924250
C	0.000000	0.000000	3.093503
C	0.000000	0.000000	1.869030
C	0.000000	1.320068	5.353511
C	0.000000	2.403234	5.924250
C	0.000000	-7.291952	6.909236
C	0.000000	-8.330800	6.276880
C	0.000000	-9.487518	5.555743
C	0.000000	-10.512456	4.901095
C	0.736323	-4.875213	7.127657
C	-0.736323	-4.875213	7.127657
C	0.736323	4.875213	7.127657
C	-0.736323	4.875213	7.127657
C	0.735893	0.000000	-0.879423
C	-0.735893	0.000000	-0.879423
B	0.000000	-15.397593	-4.875438

B	0.000000	-11.801647	1.573275
B	0.000000	-8.021664	-4.570835
C	0.000000	-11.727456	4.119682
H	0.000000	-12.636469	4.725514
C	0.000000	-17.553813	-6.202921
H	0.000000	-17.588172	-7.292880
H	0.000000	-18.542484	-5.742787
C	0.000000	-5.716004	-5.654246
H	0.000000	-5.585116	-6.738783
B	0.000000	-11.794381	-2.657026
C	0.000000	-10.454353	-3.367942
C	0.000000	-9.363256	-3.923392
C	0.000000	-11.825076	-1.140661
C	0.000000	-11.828984	0.083698
C	0.000000	-13.083369	-3.450618
C	0.000000	-14.125943	-4.092536
C	0.000000	-4.469844	-4.923317
C	0.000000	-3.421900	-4.306317
C	0.000000	-2.255408	-3.601868
C	0.000000	-1.221455	-2.962391
C	0.736026	-6.889473	-5.123643
C	-0.736026	-6.889473	-5.123643
C	0.737697	-16.467618	-5.534202
C	-0.737697	-16.467618	-5.534202
C	0.736122	-11.784399	2.832866
C	-0.736122	-11.784399	2.832866
C	0.000000	10.512456	4.901095
C	0.000000	9.487518	5.555743
C	0.000000	8.330800	6.276880
C	0.000000	7.291952	6.909236
C	0.000000	4.469844	-4.923317
C	0.000000	3.421900	-4.306317
C	0.000000	2.255408	-3.601868
C	0.000000	1.221455	-2.962391
H	0.000000	12.636469	4.725514
H	0.000000	18.542484	-5.742787

**POM-9**

E= -3603.13323561

v= 1.6799

B	-3.477550	21.798845	0.000000
B	2.525364	17.502086	0.000000
B	-4.003002	14.433871	0.000000
C	5.047533	17.143756	0.000000
H	5.751289	17.979249	0.000000
C	-4.552038	24.091658	0.000000
H	-5.631072	24.249342	0.000000
H	-3.982765	25.021763	0.000000
C	-5.338379	12.264325	0.000000
H	-6.430738	12.255900	0.000000
B	-1.679104	17.968750	0.000000
C	-2.535623	16.716746	0.000000
C	-3.209545	15.694575	0.000000
C	-0.168880	17.829174	0.000000
C	1.048209	17.695921	0.000000
C	-2.322982	19.338599	0.000000
C	-2.843389	20.446842	0.000000
C	-4.751890	10.943998	0.000000
C	-4.256422	9.833421	0.000000
C	-3.687509	8.595181	0.000000
C	-3.168401	7.495853	0.000000
C	-4.679425	13.370841	0.735985
C	-4.679425	13.370841	-0.735985
C	-4.010756	22.936640	0.737686
C	-4.010756	22.936640	-0.737686
C	3.775134	17.344130	0.736115
C	3.775134	17.344130	-0.736115
B	5.781554	1.502940	0.000000
B	0.015929	5.903608	0.000000

B	6.588538	8.933445	0.000000
C	-2.528109	6.193715	0.000000
C	6.620160	-0.901892	0.000000
H	7.684731	-1.146525	0.000000
C	7.916204	11.106771	0.000000
H	9.008417	11.120324	0.000000
B	4.218391	5.431950	0.000000
C	5.102050	6.662201	0.000000
C	5.789512	7.675321	0.000000
C	2.710755	5.598695	0.000000
C	1.493943	5.735512	0.000000
C	4.814348	4.038981	0.000000
C	5.268385	2.901972	0.000000
C	7.319683	12.422280	0.000000
C	6.808863	13.525974	0.000000
C	6.222881	14.756667	0.000000
C	5.687944	15.848869	0.000000
C	7.263250	9.996299	0.736338
C	7.263250	9.996299	-0.736338
C	6.215881	0.320938	0.736215
C	6.215881	0.320938	-0.736215
C	-1.236973	6.046201	0.735868
C	-1.236973	6.046201	-0.735868
B	-5.781554	-1.502940	0.000000
B	-0.015929	-5.903608	0.000000
B	-6.588538	-8.933445	0.000000
C	2.528109	-6.193715	0.000000
C	-6.620160	0.901892	0.000000
H	-7.684731	1.146525	0.000000
C	-7.916204	-11.106771	0.000000
H	-9.008417	-11.120324	0.000000
B	-4.218391	-5.431950	0.000000
C	-5.102050	-6.662201	0.000000
C	-5.789512	-7.675321	0.000000
C	-2.710755	-5.598695	0.000000
C	-1.493943	-5.735512	0.000000
C	-4.814348	-4.038981	0.000000
C	-5.268385	-2.901972	0.000000
C	-7.319683	-12.422280	0.000000
C	-6.808863	-13.525974	0.000000
C	-6.222881	-14.756667	0.000000
C	-5.687944	-15.848869	0.000000
C	-7.263250	-9.996299	0.736338
C	-7.263250	-9.996299	-0.736338
C	-6.215881	-0.320938	0.736215
C	-6.215881	-0.320938	-0.736215
C	1.236973	-6.046201	0.735868
C	1.236973	-6.046201	-0.735868
B	3.477550	-21.798845	0.000000
B	-2.525364	-17.502086	0.000000
B	4.003002	-14.433871	0.000000
C	-5.047533	-17.143756	0.000000
H	-5.751289	-17.979249	0.000000
C	4.552038	-24.091658	0.000000
H	5.631072	-24.249342	0.000000
H	3.982765	-25.021763	0.000000
C	5.338379	-12.264325	0.000000
H	6.430738	-12.255900	0.000000
B	1.679104	-17.968750	0.000000
C	2.535623	-16.716746	0.000000
C	3.209545	-15.694575	0.000000
C	0.168880	-17.829174	0.000000
C	-1.048209	-17.695921	0.000000
C	2.322982	-19.338599	0.000000
C	2.843389	-20.446842	0.000000
C	4.751890	-10.943998	0.000000
C	4.256422	-9.833421	0.000000
C	3.687509	-8.595181	0.000000
C	3.168401	-7.495853	0.000000

C	4.679425	-13.370841	0.735985
C	4.679425	-13.370841	-0.735985
C	4.010756	-22.936640	0.737686
C	4.010756	-22.936640	-0.737686
C	-3.775134	-17.344130	0.736115
C	-3.775134	-17.344130	-0.736115
C	-3.445015	5.068878	0.000000
C	-4.197732	4.114219	0.000000
C	-5.029140	3.034563	0.000000
C	-5.759677	2.062364	0.000000
C	5.759677	-2.062364	0.000000
C	5.029140	-3.034563	0.000000
C	4.197732	-4.114219	0.000000
C	3.445015	-5.068878	0.000000

**POM-10**

E= -4579.46249723

v= 1.1331

B	0.000000	3.731711	-4.976893
B	0.000000	0.000000	1.240861
B	0.000000	-3.731711	-4.976893
C	0.000000	0.000000	3.801426
C	0.000000	6.027534	-6.079330
H	0.000000	6.151036	-7.164654
C	0.000000	-6.027534	-6.079330
H	0.000000	-6.151036	-7.164654
B	0.000000	0.000000	-2.988019
C	0.000000	-1.318880	-3.733427
C	0.000000	-2.398564	-4.310694
C	0.000000	0.000000	-1.471221
C	0.000000	0.000000	-0.246740
C	0.000000	1.318880	-3.733427
C	0.000000	2.398564	-4.310694
C	0.000000	-7.277293	-5.355116
C	0.000000	-8.325913	-4.739298
C	0.000000	-9.492663	-4.035323
C	0.000000	-10.526177	-3.395175
C	-0.736231	-4.857706	-5.540368
C	0.736231	-4.857706	-5.540368
C	-0.736231	4.857706	-5.540368
C	0.736231	4.857706	-5.540368
C	-0.735872	0.000000	2.501881
C	0.735872	0.000000	2.501881
B	0.000000	-15.491592	6.138810
B	0.000000	-11.742823	-0.049688
B	0.000000	-8.015183	6.171526
C	0.000000	-11.746753	-2.610211
C	0.000000	-17.802146	7.209876
H	0.000000	-17.939975	8.293471
C	0.000000	-5.718409	7.272254
H	0.000000	-5.593939	8.357471
B	0.000000	-11.744932	4.179152
C	0.000000	-10.427449	4.927446
C	0.000000	-9.348232	5.505553
C	0.000000	-11.741440	2.662327
C	0.000000	-11.741105	1.437854
C	0.000000	-13.066687	4.918936
C	0.000000	-14.150961	5.487585
C	0.000000	-4.469060	6.546875
C	0.000000	-3.420851	5.930352
C	0.000000	-2.254545	5.225642
C	0.000000	-1.221238	4.585152
C	-0.736183	-6.888482	6.734096
C	0.736183	-6.888482	6.734096
C	-0.736353	-16.624547	6.687699
C	0.736353	-16.624547	6.687699
C	-0.735887	-11.744567	-1.310677
C	0.735887	-11.744567	-1.310677
B	0.000000	-19.769192	-5.007888
B	0.000000	-23.551472	1.132335

B	0.000000	-27.147593	-5.315378
C	0.000000	-23.477203	3.678761
C	0.000000	-17.461636	-6.087357
H	0.000000	-17.329020	-7.171694
C	0.000000	-29.305111	-6.640746
H	0.000000	-29.340606	-7.730657
B	0.000000	-23.543824	-3.097935
C	0.000000	-24.832592	-3.891766
C	0.000000	-25.875363	-4.533355
C	0.000000	-23.574770	-1.581585
C	0.000000	-23.578723	-0.357234
C	0.000000	-22.203389	-3.808183
C	0.000000	-21.111678	-4.362403
C	-0.737702	-28.218220	-5.973134
C	0.737702	-28.218220	-5.973134
C	-0.735999	-18.635883	-5.558554
C	0.735999	-18.635883	-5.558554
C	-0.736121	-23.534130	2.391940
C	0.736121	-23.534130	2.391940
C	0.000000	-12.968950	-3.392333
C	0.000000	-14.002889	-4.031828
C	0.000000	-15.168979	-4.736916
C	0.000000	-16.216440	-5.354724
C	0.000000	-19.041330	6.467693
C	0.000000	-20.080302	5.835548
C	0.000000	-21.237014	5.114418
C	0.000000	-22.262084	4.459985
B	0.000000	8.015183	6.171526
B	0.000000	15.491592	6.138810
B	0.000000	11.742823	-0.049688
C	0.000000	17.802146	7.209876
H	0.000000	17.939975	8.293471
C	0.000000	5.718409	7.272254
H	0.000000	5.593939	8.357471
C	0.000000	11.746753	-2.610211
B	0.000000	11.744932	4.179152
C	0.000000	11.741440	2.662327
C	0.000000	11.741105	1.437854
C	0.000000	13.066687	4.918936
C	0.000000	14.150961	5.487585
C	0.000000	10.427449	4.927446
C	0.000000	9.348232	5.505553
C	0.000000	12.968950	-3.392333
C	0.000000	14.002889	-4.031828
C	0.000000	15.168979	-4.736916
C	0.000000	16.216440	-5.354724
C	0.735887	11.744567	-1.310677
C	-0.735887	11.744567	-1.310677
C	0.736183	6.888482	6.734096
C	-0.736183	6.888482	6.734096
C	0.736353	16.624547	6.687699
C	-0.736353	16.624547	6.687699
B	0.000000	27.147593	-5.315378
B	0.000000	19.769192	-5.007888
B	0.000000	23.551472	1.132335
C	0.000000	17.461636	-6.087357
H	0.000000	17.329020	-7.171694
C	0.000000	29.305111	-6.640746
H	0.000000	30.292916	-6.180021
H	0.000000	29.340606	-7.730657
C	0.000000	23.477203	3.678761
H	0.000000	24.386292	4.284538
B	0.000000	23.543824	-3.097935
C	0.000000	23.574770	-1.581585
C	0.000000	23.578723	-0.357234
C	0.000000	22.203389	-3.808183
C	0.000000	21.111678	-4.362403
C	0.000000	24.832592	-3.891766
C	0.000000	25.875363	-4.533355

C	0.000000	22.262084	4.459985
C	0.000000	21.237014	5.114418
C	0.000000	20.080302	5.835548
C	0.000000	19.041330	6.467693
C	0.736121	23.534130	2.391940
C	-0.736121	23.534130	2.391940
C	0.737702	28.218220	-5.973134
C	-0.737702	28.218220	-5.973134
C	0.735999	18.635883	-5.558554
C	-0.735999	18.635883	-5.558554
C	0.000000	1.221238	4.585152
C	0.000000	2.254545	5.225642
C	0.000000	3.420851	5.930352
C	0.000000	4.469060	6.546875
C	0.000000	7.277293	-5.355116
C	0.000000	8.325913	-4.739298
C	0.000000	9.492663	-4.035323
C	0.000000	10.526177	-3.395175
H	0.000000	-24.386292	4.284538
H	0.000000	-30.292916	-6.180021

**POM-11**

E= -5555.79171690

v= 0.7555

B	-5.132576	9.848442	0.000000
B	0.911215	5.839535	0.000000
B	-5.468236	2.392894	0.000000
C	3.469073	5.722545	0.000000
C	-6.130953	12.191359	0.000000
H	-7.209616	12.363546	0.000000
C	-6.673458	0.149315	0.000000
H	-7.763250	0.074969	0.000000
B	-3.313301	6.031220	0.000000
C	-4.117326	4.747123	0.000000
C	-4.742611	3.694519	0.000000
C	-1.798057	5.962742	0.000000
C	-0.574831	5.907226	0.000000
C	-3.998613	7.382310	0.000000
C	-4.526859	8.486813	0.000000
C	-6.006298	-1.132029	0.000000
C	-5.438604	-2.207463	0.000000
C	-4.788380	-3.404999	0.000000
C	-4.196078	-4.466659	0.000000
C	-6.082061	1.293408	0.736213
C	-6.082061	1.293408	-0.736213
C	-5.645085	10.998582	0.736237
C	-5.645085	10.998582	-0.736237
C	2.170899	5.781911	0.735866
C	2.170899	5.781911	-0.735866
B	5.132576	-9.848442	0.000000
B	-0.911215	-5.839535	0.000000
B	5.468236	-2.392894	0.000000
C	-3.469073	-5.722545	0.000000
C	6.130953	-12.191359	0.000000
H	7.209616	-12.363546	0.000000
C	6.673458	-0.149315	0.000000
H	7.763250	-0.074969	0.000000
B	3.313301	-6.031220	0.000000
C	4.117326	-4.747123	0.000000
C	4.742611	-3.694519	0.000000
C	1.798057	-5.962742	0.000000
C	0.574831	-5.907226	0.000000
C	3.998613	-7.382310	0.000000
C	4.526859	-8.486813	0.000000
C	6.006298	1.132029	0.000000
C	5.438604	2.207463	0.000000
C	4.788380	3.404999	0.000000
C	4.196078	4.466659	0.000000
C	6.082061	-1.293408	0.736213

C	6.082061	-1.293408	-0.736213
C	5.645085	-10.998582	0.736237
C	5.645085	-10.998582	-0.736237
C	-2.170899	-5.781911	0.735866
C	-2.170899	-5.781911	-0.735866
B	-6.199746	-13.620606	0.000000
B	-0.152685	-17.626304	0.000000
B	-6.506646	-21.089151	0.000000
C	2.404981	-17.746860	0.000000
C	-7.196719	-11.276956	0.000000
H	-8.275230	-11.103805	0.000000
C	-7.683627	-23.347558	0.000000
H	-8.772422	-23.435215	0.000000
B	-4.377253	-17.436268	0.000000
C	-5.176481	-18.722940	0.000000
C	-5.794314	-19.779968	0.000000
C	-2.861833	-17.501653	0.000000
C	-1.638605	-17.556942	0.000000
C	-5.065147	-16.086248	0.000000
C	-5.594188	-14.982147	0.000000
C	-6.999300	-24.619600	0.000000
C	-6.415330	-25.686395	0.000000
C	-5.748151	-26.875045	0.000000
C	-5.141386	-27.929032	0.000000
C	-7.107586	-22.195349	0.736356
C	-7.107586	-22.195349	-0.736356
C	-6.711598	-12.469985	0.736184
C	-6.711598	-12.469985	-0.736184
C	1.106903	-17.685475	0.735880
C	1.106903	-17.685475	-0.735880
B	4.404270	-33.252815	0.000000
B	-1.876254	-29.369294	0.000000
B	4.430655	-25.870262	0.000000
C	-4.416587	-29.178642	0.000000
H	-5.063497	-30.058894	0.000000
C	5.633387	-35.466548	0.000000
H	6.720693	-35.549911	0.000000
H	5.129220	-36.433502	0.000000
C	5.616094	-23.615333	0.000000
H	6.705403	-23.533067	0.000000
B	2.350006	-29.553597	0.000000
C	3.120303	-28.246732	0.000000
C	3.723935	-27.181541	0.000000
C	0.833804	-29.515931	0.000000
C	-0.389473	-29.464382	0.000000
C	3.084899	-30.876861	0.000000
C	3.679333	-31.947222	0.000000
C	4.941808	-22.337597	0.000000
C	4.372851	-21.262818	0.000000
C	3.722196	-20.065497	0.000000
C	3.130643	-19.003398	0.000000
C	5.033427	-24.763799	0.736004
C	5.033427	-24.763799	-0.736004
C	5.014222	-34.351361	0.737705
C	5.014222	-34.351361	-0.737705
C	-3.133740	-29.294457	0.736119
C	-3.133740	-29.294457	-0.736119
C	-4.307908	-6.906626	0.000000
C	-4.994955	-7.909581	0.000000
C	-5.752045	-9.042587	0.000000
C	-6.415719	-10.061595	0.000000
C	5.350894	-13.407240	0.000000
C	4.687972	-14.426740	0.000000
C	3.931465	-15.560139	0.000000
C	3.244751	-16.563319	0.000000
B	6.199746	13.620606	0.000000
B	6.506646	21.089151	0.000000
B	0.152685	17.626304	0.000000
C	7.683627	23.347558	0.000000

H	8.772422	23.435215	0.000000
C	7.196719	11.276956	0.000000
H	8.275230	11.103805	0.000000
C	-2.404981	17.746860	0.000000
B	4.377253	17.436268	0.000000
C	2.861833	17.501653	0.000000
C	1.638605	17.556942	0.000000
C	5.176481	18.722940	0.000000
C	5.794314	19.779968	0.000000
C	5.065147	16.086248	0.000000
C	5.594188	14.982147	0.000000
C	-3.130643	19.003398	0.000000
C	-3.722196	20.065497	0.000000
C	-4.372851	21.262818	0.000000
C	-4.941808	22.337597	0.000000
C	-1.106903	17.685475	-0.735880
C	-1.106903	17.685475	0.735880
C	6.711598	12.469985	-0.736184
C	6.711598	12.469985	0.736184
C	7.107586	22.195349	-0.736356
C	7.107586	22.195349	0.736356
B	-4.404270	33.252815	0.000000
B	-4.430655	25.870262	0.000000
B	1.876254	29.369294	0.000000
C	-5.616094	23.615333	0.000000
H	-6.705403	23.533067	0.000000
C	-5.633387	35.466548	0.000000
H	-5.129220	36.433502	0.000000
H	-6.720693	35.549911	0.000000
C	4.416587	29.178642	0.000000
H	5.063497	30.058894	0.000000
B	-2.350006	29.553597	0.000000
C	-0.833804	29.515931	0.000000
C	0.389473	29.464382	0.000000
C	-3.120303	28.246732	0.000000
C	-3.723935	27.181541	0.000000
C	-3.084899	30.876861	0.000000
C	-3.679333	31.947222	0.000000
C	5.141386	27.929032	0.000000
C	5.748151	26.875045	0.000000
C	6.415330	25.686395	0.000000
C	6.999300	24.619600	0.000000
C	3.133740	29.294457	-0.736119
C	3.133740	29.294457	0.736119
C	-5.014222	34.351361	-0.737705
C	-5.014222	34.351361	0.737705
C	-5.033427	24.763799	-0.736004
C	-5.033427	24.763799	0.736004
C	4.307908	6.906626	0.000000
C	4.994955	7.909581	0.000000
C	5.752045	9.042587	0.000000
C	6.415719	10.061595	0.000000
C	-5.350894	13.407240	0.000000
C	-4.687972	14.426740	0.000000
C	-3.931465	15.560139	0.000000
C	-3.244751	16.563319	0.000000

**POM-12**

E= -3603.12872390

v= 3.2527

B	-3.635024	-11.424309	0.000000
B	3.635024	-11.424309	0.000000
B	0.000000	-17.820900	0.000000
C	5.799266	-10.079980	0.000000
C	-5.799266	-10.079980	0.000000
H	-6.780193	-10.560584	0.000000
C	0.000000	-20.352991	0.000000
H	-0.910166	-20.953641	0.000000
B	0.000000	-13.589356	0.000000
C	0.000000	-15.103174	0.000000

C	0.000000	-16.327542	0.000000
C	1.310671	-12.825714	0.000000
C	2.364198	-12.201872	0.000000
C	-1.310671	-12.825714	0.000000
C	-2.364198	-12.201872	0.000000
C	0.000000	-19.077422	0.737699
C	0.000000	-19.077422	-0.737699
C	-4.715132	-10.775404	0.735989
C	-4.715132	-10.775404	-0.735989
C	4.715132	-10.775404	0.735989
C	4.715132	-10.775404	-0.735989
B	3.660566	-2.113429	0.000000
B	-3.660566	-2.113429	0.000000
B	0.000000	4.226857	0.000000
C	-5.877541	-3.393400	0.000000
C	5.877541	-3.393400	0.000000
C	0.000000	6.786799	0.000000
B	0.000000	0.000000	0.000000
C	0.000000	1.514982	0.000000
C	0.000000	2.739296	0.000000
C	-1.312013	-0.757491	0.000000
C	-2.372300	-1.369648	0.000000
C	1.312013	-0.757491	0.000000
C	2.372300	-1.369648	0.000000
C	-1.226063	7.562778	0.000000
C	-2.280564	8.167779	0.000000
C	-3.473190	8.826984	0.000000
C	-4.547946	9.396005	0.000000
C	0.000000	5.487150	0.736115
C	0.000000	5.487150	-0.736115
C	4.752012	-2.743575	0.736115
C	4.752012	-2.743575	-0.736115
C	-4.752012	-2.743575	0.736115
C	-4.752012	-2.743575	-0.736115
B	-15.433352	8.910450	0.000000
B	-8.076230	8.860177	0.000000
B	-11.711253	2.564132	0.000000
C	-5.829886	10.062302	0.000000
H	-5.755638	11.152112	0.000000
C	-17.626208	10.176496	0.000000
H	-18.601468	9.688594	0.000000
H	-17.691302	11.265047	0.000000
C	-11.629152	0.017678	0.000000
H	-12.535831	-0.591527	0.000000
B	-11.768727	6.794678	0.000000
C	-11.762730	5.277783	0.000000
C	-11.749230	4.053481	0.000000
C	-10.452059	7.547931	0.000000
C	-9.385033	8.148391	0.000000
C	-13.079732	7.551587	0.000000
C	-14.140066	8.163771	0.000000
C	-10.411153	-0.759366	0.000000
C	-9.380987	-1.405621	0.000000
C	-8.213786	-2.108864	0.000000
C	-7.162589	-2.719588	0.000000
C	-11.689340	1.304278	0.735989
C	-11.689340	1.304278	-0.735989
C	-16.521533	9.538711	0.737699
C	-16.521533	9.538711	-0.737699
C	-6.974207	9.471126	0.735989
C	-6.974207	9.471126	-0.735989
B	8.076230	8.860177	0.000000
B	15.433352	8.910450	0.000000
B	11.711253	2.564132	0.000000
C	17.626208	10.176496	0.000000
H	17.691302	11.265047	0.000000
C	5.829886	10.062302	0.000000
H	5.755638	11.152112	0.000000
C	11.629152	0.017678	0.000000

B	11.768727	6.794678	0.000000
C	11.762730	5.277783	0.000000
C	11.749230	4.053481	0.000000
C	13.079732	7.551587	0.000000
C	14.140066	8.163771	0.000000
C	10.452059	7.547931	0.000000
C	9.385033	8.148391	0.000000
C	11.689340	1.304278	0.735989
C	11.689340	1.304278	-0.735989
C	6.974207	9.471126	0.735989
C	6.974207	9.471126	-0.735989
C	16.521533	9.538711	0.737699
C	16.521533	9.538711	-0.737699
C	5.863206	-8.636640	0.000000
C	5.907797	-7.421362	0.000000
C	5.933222	-6.058915	0.000000
C	5.936527	-4.843190	0.000000
C	-5.936527	-4.843190	0.000000
C	-5.933222	-6.058915	0.000000
C	-5.907797	-7.421362	0.000000
C	-5.863206	-8.636640	0.000000
C	10.411153	-0.759366	0.000000
C	9.380987	-1.405621	0.000000
C	8.213786	-2.108864	0.000000
C	7.162589	-2.719588	0.000000
C	4.547946	9.396005	0.000000
C	3.473190	8.826984	0.000000
C	2.280564	8.167779	0.000000
C	1.226063	7.562778	0.000000
H	0.910166	-20.953641	0.000000
H	6.780193	-10.560584	0.000000
H	12.535831	-0.591527	0.000000
H	18.601468	9.688594	0.000000

**POM-13**

E= -2259.75160921  
 v= 2.6087

B	-16.448545	0.000000	0.000000
B	-6.048811	5.780537	0.000000
B	-6.048811	-5.780537	0.000000
C	-4.629845	7.896956	0.000000
H	-5.078454	8.893220	0.000000
C	-18.980348	0.000000	0.000000
H	-19.581124	-0.910125	0.000000
H	-19.581124	0.910125	0.000000
C	-4.629845	-7.896956	0.000000
H	-5.078454	-8.893220	0.000000
C	-7.521396	-3.504148	0.000000
C	-6.867380	-4.540050	0.000000
C	-7.521396	3.504148	0.000000
C	-6.867380	4.540050	0.000000
C	-14.958593	0.000000	0.000000
C	-3.186432	-7.914914	0.000000
C	-1.968011	-7.932382	0.000000
C	-0.612632	-7.943721	0.000000
C	-5.362501	-6.837470	0.736619
C	-5.362501	-6.837470	-0.736619
C	-17.705346	0.000000	0.738402
C	-17.705346	0.000000	-0.738402
C	-5.362501	6.837470	0.736619
C	-5.362501	6.837470	-0.736619
B	16.448545	0.000000	0.000000
B	6.048811	-5.780537	0.000000
B	6.048811	5.780537	0.000000
C	4.629845	-7.896956	0.000000
H	5.078454	-8.893220	0.000000
C	18.980348	0.000000	0.000000
H	19.581124	0.910125	0.000000
H	19.581124	-0.910125	0.000000

C	4.629845	7.896956	0.000000
H	5.078454	8.893220	0.000000
C	7.521396	3.504148	0.000000
C	6.867380	4.540050	0.000000
C	7.521396	-3.504148	0.000000
C	6.867380	-4.540050	0.000000
C	14.958593	0.000000	0.000000
C	0.612632	7.943721	0.000000
C	-0.612632	7.943721	0.000000
C	-1.968011	7.932382	0.000000
C	-3.186432	7.914914	0.000000
C	5.362501	6.837470	0.736619
C	5.362501	6.837470	-0.736619
C	17.705346	0.000000	0.738402
C	17.705346	0.000000	-0.738402
C	5.362501	-6.837470	0.736619
C	5.362501	-6.837470	-0.736619
B	9.640484	0.000000	0.000000
B	-9.640484	0.000000	0.000000
C	-8.875306	1.305167	0.000000
C	-8.236792	2.353803	0.000000
C	-8.875306	-1.305167	0.000000
C	-8.236792	-2.353803	0.000000
C	8.875306	1.305167	0.000000
C	8.236792	2.353803	0.000000
C	8.875306	-1.305167	0.000000
C	8.236792	-2.353803	0.000000
C	0.612632	-7.943721	0.000000
C	1.968011	7.932382	0.000000
C	3.186432	7.914914	0.000000
C	1.968011	-7.932382	0.000000
C	3.186432	-7.914914	0.000000
C	13.733702	0.000000	0.000000
C	12.378729	0.000000	0.000000
C	11.150835	0.000000	0.000000
C	-13.733702	0.000000	0.000000
C	-12.378729	0.000000	0.000000
C	-11.150835	0.000000	0.000000

**POM-14**

E= -3616.87806137

v= 1.8350

B	0.000000	10.224868	-6.789144
B	0.000000	16.289163	3.089113
C	0.000000	16.210104	5.635946
C	0.000000	7.916802	-7.868874
H	0.000000	7.786247	-8.953670
C	0.000000	16.335098	0.378320
C	0.000000	16.326517	1.603381
C	0.000000	11.566969	-6.151146
C	0.736555	9.090768	-7.339217
C	-0.736555	9.090768	-7.339217
C	0.736643	16.268358	4.349187
C	-0.736643	16.268358	4.349187
B	0.000000	16.297437	-3.716589
C	0.000000	16.328495	-2.204063
C	0.000000	16.336726	-0.976344
C	0.000000	12.663535	-5.604893
C	0.000000	13.872416	-4.993550
C	0.000000	14.963327	-4.430334
B	0.000000	6.033301	9.453137
B	0.000000	0.000000	-0.494801
B	0.000000	-6.033301	9.453137
C	0.000000	0.000000	-3.056715
C	0.000000	8.345418	10.522721
H	0.000000	8.481943	11.606718
C	0.000000	-8.345418	10.522721
H	0.000000	-8.481943	11.606718
C	0.000000	-3.598937	8.258934

C	0.000000	-4.691169	8.813686
C	0.000000	0.000000	2.214032
C	0.000000	0.000000	0.988695
C	0.000000	4.691169	8.813686
C	0.000000	-9.585656	9.784221
C	0.000000	-10.630928	9.157932
C	0.000000	-11.788676	8.453122
C	0.736800	-7.168060	10.000004
C	-0.736800	-7.168060	10.000004
C	0.736800	7.168060	10.000004
C	-0.736800	7.168060	10.000004
C	0.736312	0.000000	-1.756770
C	-0.736312	0.000000	-1.756770
B	0.000000	-22.106006	-7.267741
B	0.000000	-16.289163	3.089113
B	0.000000	-10.224868	-6.789144
C	0.000000	-16.210104	5.635946
C	0.000000	-24.267560	-8.585898
H	0.000000	-24.306585	-9.675743
C	0.000000	-7.916802	-7.868874
H	0.000000	-7.786247	-8.953670
C	0.000000	-12.663535	-5.604893
C	0.000000	-11.566969	-6.151146
C	0.000000	-16.335098	0.378320
C	0.000000	-16.326517	1.603381
C	0.000000	-20.834136	-6.491594
C	0.000000	-4.451372	-5.836745
C	0.000000	-3.402496	-5.203300
C	0.000000	-2.250071	-4.490821
C	0.000000	-1.219255	-3.841661
C	0.736555	-9.090768	-7.339217
C	-0.736555	-9.090768	-7.339217
C	0.738417	-23.179040	-7.922007
C	-0.738417	-23.179040	-7.922007
C	0.736643	-16.268358	4.349187
C	-0.736643	-16.268358	4.349187
B	0.000000	-16.297437	-3.716589
B	0.000000	0.000000	6.309021
C	0.000000	0.000000	4.795946
C	0.000000	0.000000	3.568164
C	0.000000	-1.315022	7.053977
C	0.000000	-2.397122	7.634066
C	0.000000	-14.963327	-4.430334
C	0.000000	-13.872416	-4.993550
C	0.000000	-16.328495	-2.204063
C	0.000000	-16.336726	-0.976344
C	0.000000	-12.828814	7.805406
C	0.000000	-5.618088	-6.526195
C	0.000000	-6.670887	-7.139682
C	0.000000	-13.972493	7.077993
C	0.000000	-14.996506	6.417523
C	0.000000	-19.788781	-5.853245
C	0.000000	-18.632598	-5.146715
C	0.000000	-17.585180	-4.505888
C	0.000000	3.598937	8.258934
C	0.000000	2.397122	7.634066
C	0.000000	1.315022	7.053977
C	0.000000	1.219255	-3.841661
C	0.000000	2.250071	-4.490821
C	0.000000	3.402496	-5.203300
C	0.000000	4.451372	-5.836745
C	0.000000	5.618088	-6.526195
C	0.000000	6.670887	-7.139682
C	0.000000	9.585656	9.784221
C	0.000000	10.630928	9.157932
C	0.000000	11.788676	8.453122
C	0.000000	12.828814	7.805406
C	0.000000	13.972493	7.077993
C	0.000000	14.996506	6.417523

H	0.000000	17.119179	6.242046
B	0.000000	22.106006	-7.267741
C	0.000000	19.788781	-5.853245
C	0.000000	20.834136	-6.491594
C	0.738417	23.179040	-7.922007
C	-0.738417	23.179040	-7.922007
C	0.000000	17.585180	-4.505888
C	0.000000	18.632598	-5.146715
C	0.000000	24.267560	-8.585898
H	0.000000	24.306585	-9.675743
H	0.000000	25.254346	-8.121799
H	0.000000	-17.119179	6.242046
H	0.000000	-25.254346	-8.121799

**POM-15**

E= -4974.00448166

v= 0.8122

B	6.115824	19.112528	0.000000
B	-4.363485	24.074616	0.000000
C	-6.886879	23.721089	0.000000
C	7.442212	16.936786	0.000000
H	8.534757	16.925778	0.000000
C	-1.673414	24.412234	0.000000
C	-2.890428	24.271827	0.000000
C	5.334936	20.376827	0.000000
C	6.787109	18.045655	0.736521
C	6.787109	18.045655	-0.736521
C	-5.613953	23.917920	0.736638
C	-5.613953	23.917920	-0.736638
B	2.401811	24.815519	0.000000
C	0.894687	24.683529	0.000000
C	-0.326788	24.559669	0.000000
C	4.672514	21.407378	0.000000
C	3.933345	22.542637	0.000000
C	3.255242	23.566085	0.000000
B	-9.567068	13.189529	0.000000
B	0.974696	8.263700	0.000000
B	-8.313918	1.212876	0.000000
C	3.521344	8.542803	0.000000
C	-10.885064	15.369620	0.000000
H	-11.977480	15.385772	0.000000
C	-9.158278	-1.190736	0.000000
H	-10.224194	-1.430513	0.000000
C	-7.362831	3.751887	0.000000
C	-7.807169	2.610273	0.000000
C	-1.718132	7.969438	0.000000
C	-0.500004	8.102177	0.000000
C	-8.784410	11.925568	0.000000
C	-8.304987	-2.355140	0.000000
C	-7.582382	-3.336246	0.000000
C	-6.771500	-4.422092	0.000000
C	-8.749752	0.030692	0.736718
C	-8.749752	0.030692	-0.736718
C	-10.235823	14.257038	0.736801
C	-10.235823	14.257038	-0.736801
C	2.229200	8.400927	0.736295
C	2.229200	8.400927	-0.736295
B	9.567068	-13.189529	0.000000
B	-0.974696	-8.263700	0.000000
B	8.313918	-1.212876	0.000000
C	-3.521344	-8.542803	0.000000
C	10.885064	-15.369620	0.000000
H	11.977480	-15.385772	0.000000
C	9.158278	1.190736	0.000000
H	10.224194	1.430513	0.000000
C	7.362831	-3.751887	0.000000
C	7.807169	-2.610273	0.000000
C	1.718132	-7.969438	0.000000
C	0.500004	-8.102177	0.000000
C	8.784410	-11.925568	0.000000

C	6.771500	4.422092	0.000000
C	6.028053	5.396084	0.000000
C	5.193609	6.463525	0.000000
C	4.434937	7.416610	0.000000
C	8.749752	-0.030692	0.736718
C	8.749752	-0.030692	-0.736718
C	10.235823	-14.257038	0.736801
C	10.235823	-14.257038	-0.736801
C	-2.229200	-8.400927	0.736295
C	-2.229200	-8.400927	-0.736295
B	5.789518	-7.531014	0.000000
B	-5.789518	7.531014	0.000000
C	-4.285037	7.691303	0.000000
C	-3.064356	7.823183	0.000000
C	-6.393080	6.145169	0.000000
C	-6.860791	5.009993	0.000000
C	6.393080	-6.145169	0.000000
C	6.860791	-5.009993	0.000000
C	4.285037	-7.691303	0.000000
C	3.064356	-7.823183	0.000000
C	-6.028053	-5.396084	0.000000
C	7.582382	3.336246	0.000000
C	8.304987	2.355140	0.000000
C	-5.193609	-6.463525	0.000000
C	-4.434937	-7.416610	0.000000
C	8.114242	-10.900042	0.000000
C	7.362895	-9.772976	0.000000
C	6.669738	-8.759561	0.000000
C	-8.114242	10.900042	0.000000
C	-7.362895	9.772976	0.000000
C	-6.669738	8.759561	0.000000
C	4.168952	9.840217	0.000000
C	4.702391	10.935405	0.000000
C	5.285307	12.158480	0.000000
C	5.800465	13.270242	0.000000
C	6.358601	14.505173	0.000000
C	6.853749	15.618531	0.000000
C	-10.287672	16.683627	0.000000
C	-9.779781	17.791270	0.000000
C	-9.206349	19.019403	0.000000
C	-8.676363	20.124188	0.000000
C	-8.078031	21.340388	0.000000
C	-7.532794	22.430126	0.000000
B	-6.115824	-19.112528	0.000000
B	4.363485	-24.074616	0.000000
B	-5.309414	-30.971404	0.000000
C	6.886879	-23.721089	0.000000
C	-7.442212	-16.936786	0.000000
H	-8.534757	-16.925778	0.000000
C	-6.388506	-33.261640	0.000000
H	-7.467896	-33.417231	0.000000
C	-4.151089	-28.516047	0.000000
C	-4.673949	-29.623708	0.000000
C	1.673414	-24.412234	0.000000
C	2.890428	-24.271827	0.000000
C	-5.334936	-20.376827	0.000000
C	-5.845067	-32.108273	0.738427
C	-5.845067	-32.108273	-0.738427
C	-6.787109	-18.045655	0.736521
C	-6.787109	-18.045655	-0.736521
C	5.613953	-23.917920	0.736638
C	5.613953	-23.917920	-0.736638
B	-2.401811	-24.815519	0.000000
C	-0.894687	-24.683529	0.000000
C	0.326788	-24.559669	0.000000
C	-3.047765	-26.180701	0.000000
C	-3.572417	-27.290890	0.000000
C	-4.672514	-21.407378	0.000000
C	-3.933345	-22.542637	0.000000

C	-3.255242	-23.566085	0.000000
C	7.532794	-22.430126	0.000000
C	8.078031	-21.340388	0.000000
C	8.676363	-20.124188	0.000000
C	9.206349	-19.019403	0.000000
C	9.779781	-17.791270	0.000000
C	10.287672	-16.683627	0.000000
C	-6.853749	-15.618531	0.000000
C	-6.358601	-14.505173	0.000000
C	-5.800465	-13.270242	0.000000
C	-5.285307	-12.158480	0.000000
C	-4.702391	-10.935405	0.000000
C	-4.168952	-9.840217	0.000000
H	-7.587713	24.559316	0.000000
B	5.309414	30.971404	0.000000
C	4.151089	28.516047	0.000000
C	4.673949	29.623708	0.000000
C	5.845067	32.108273	0.738427
C	5.845067	32.108273	-0.738427
C	3.047765	26.180701	0.000000
C	3.572417	27.290890	0.000000
C	6.388506	33.261640	0.000000
H	7.467896	33.417231	0.000000
H	5.821457	34.193006	0.000000
H	-5.821457	-34.193006	0.000000
H	7.587713	-24.559316	0.000000

**POM-16**

E= -6331.13091719

v= 0.6271

B	0.000000	26.460485	-7.369566
B	0.000000	32.528411	2.505732
C	0.000000	32.448706	5.052540
C	0.000000	24.151810	-8.448013
H	0.000000	24.020576	-9.532723
C	0.000000	32.574035	-0.205057
C	0.000000	32.565701	1.020003
C	0.000000	27.802897	-6.732286
C	0.736531	25.326029	-7.918981
C	-0.736531	25.326029	-7.918981
C	0.736637	32.507329	3.765806
C	-0.736637	32.507329	3.765806
B	0.000000	32.534578	-4.299979
C	0.000000	32.566408	-2.787436
C	0.000000	32.575201	-1.559726
C	0.000000	28.899746	-6.186608
C	0.000000	30.108895	-5.575781
C	0.000000	31.200067	-5.013089
B	0.000000	22.268763	8.865182
B	0.000000	16.230579	-1.075130
B	0.000000	10.220087	8.915157
C	0.000000	16.234206	-3.637035
C	0.000000	24.580977	9.934461
H	0.000000	24.717401	11.018466
C	0.000000	7.920418	10.011579
H	0.000000	7.796319	11.097070
C	0.000000	12.643038	7.698484
C	0.000000	11.555360	8.262110
C	0.000000	16.227919	1.633721
C	0.000000	16.228678	0.408383
C	0.000000	20.926340	8.226376
C	0.000000	6.671034	9.288392
C	0.000000	5.617433	8.676309
C	0.000000	4.450185	7.987758
C	0.736671	9.091040	9.474513
C	-0.736671	9.091040	9.474513
C	0.736816	23.403643	9.411817
C	-0.736816	23.403643	9.411817
C	0.736305	16.232282	-2.337110
C	-0.736305	16.232282	-2.337110

B	0.000000	-6.013647	-7.342335
B	0.000000	0.000000	2.643809
B	0.000000	6.013647	-7.342335
C	0.000000	0.000000	5.205724
C	0.000000	-8.312375	-8.440568
H	0.000000	-8.435323	-9.526183
C	0.000000	8.312375	-8.440568
H	0.000000	8.435323	-9.526183
C	0.000000	3.590954	-6.125151
C	0.000000	4.678725	-6.688605
C	0.000000	0.000000	-0.065077
C	0.000000	0.000000	1.160266
C	0.000000	-4.678725	-6.688605
C	0.000000	11.784299	-6.419437
C	0.000000	12.833551	-5.786630
C	0.000000	13.985721	-5.073734
C	0.000000	15.015868	-4.423542
C	0.736698	7.142306	-7.902415
C	-0.736698	7.142306	-7.902415
C	0.736698	-7.142306	-7.902415
C	-0.736698	-7.142306	-7.902415
C	0.736294	0.000000	3.905807
C	-0.736294	0.000000	3.905807
B	0.000000	0.000000	-4.160001
B	0.000000	16.231500	5.728667
C	0.000000	16.228218	4.215646
C	0.000000	16.227639	2.987862
C	0.000000	14.918781	6.478162
C	0.000000	13.840231	7.064761
C	0.000000	1.314189	-4.906734
C	0.000000	2.393345	-5.492263
C	0.000000	0.000000	-2.647024
C	0.000000	0.000000	-1.419233
C	0.000000	3.401189	7.354526
C	0.000000	10.616574	-7.107185
C	0.000000	9.562472	-7.718403
C	0.000000	2.249311	6.641160
C	0.000000	1.219150	5.990985
C	0.000000	-3.590954	-6.125151
C	0.000000	-2.393345	-5.492263
C	0.000000	-1.314189	-4.906734
C	0.000000	19.833547	7.672735
C	0.000000	18.631068	7.049189
C	0.000000	17.548099	6.470683
C	0.000000	17.454241	-4.420708
C	0.000000	18.485325	-5.069440
C	0.000000	19.637899	-5.781690
C	0.000000	20.687047	-6.414684
C	0.000000	21.853650	-7.104341
C	0.000000	22.906234	-7.718182
C	0.000000	25.821279	9.196119
C	0.000000	26.866817	8.570279
C	0.000000	28.025251	7.866583
C	0.000000	29.066026	7.219886
C	0.000000	30.210355	6.493471
C	0.000000	31.234789	5.833666
B	0.000000	-10.220087	8.915157
B	0.000000	-16.230579	-1.075130
B	0.000000	-22.268763	8.865182
C	0.000000	-16.234206	-3.637035
C	0.000000	-7.920418	10.011579
H	0.000000	-7.796319	11.097070
C	0.000000	-24.580977	9.934461
H	0.000000	-24.717401	11.018466
C	0.000000	-19.833547	7.672735
C	0.000000	-20.926340	8.226376
C	0.000000	-16.227919	1.633721
C	0.000000	-16.228678	0.408383
C	0.000000	-11.555360	8.262110



C	0.000000	-25.821279	9.196119
C	0.000000	-26.866817	8.570279
C	0.000000	-28.025251	7.866583
C	0.736816	-23.403643	9.411817
C	-0.736816	-23.403643	9.411817
C	0.736671	-9.091040	9.474513
C	-0.736671	-9.091040	9.474513
C	0.736305	-16.232282	-2.337110
C	-0.736305	-16.232282	-2.337110
B	0.000000	-38.340795	-7.854950
B	0.000000	-32.528411	2.505732
B	0.000000	-26.460485	-7.369566
C	0.000000	-32.448706	5.052540
C	0.000000	-40.501351	-9.174679
H	0.000000	-40.539815	-10.264534
C	0.000000	-24.151810	-8.448013
H	0.000000	-24.020576	-9.532723
C	0.000000	-28.899746	-6.186608
C	0.000000	-27.802897	-6.732286
C	0.000000	-32.574035	-0.205057
C	0.000000	-32.565701	1.020003
C	0.000000	-37.069533	-7.077765
C	0.000000	-20.687047	-6.414684
C	0.000000	-19.637899	-5.781690
C	0.000000	-18.485325	-5.069440
C	0.000000	-17.454241	-4.420708
C	0.736531	-25.326029	-7.918981
C	-0.736531	-25.326029	-7.918981
C	0.738424	-39.413230	-8.510149
C	-0.738424	-39.413230	-8.510149
C	0.736637	-32.507329	3.765806
C	-0.736637	-32.507329	3.765806
B	0.000000	-32.534578	-4.299979
B	0.000000	-16.231500	5.728667
C	0.000000	-16.228218	4.215646
C	0.000000	-16.227639	2.987862
C	0.000000	-17.548099	6.470683
C	0.000000	-18.631068	7.049189
C	0.000000	-31.200067	-5.013089
C	0.000000	-30.108895	-5.575781
C	0.000000	-32.566408	-2.787436
C	0.000000	-32.575201	-1.559726
C	0.000000	-29.066026	7.219886
C	0.000000	-21.853650	-7.104341
C	0.000000	-22.906234	-7.718182
C	0.000000	-30.210355	6.493471
C	0.000000	-31.234789	5.833666
C	0.000000	-36.024770	-6.438418
C	0.000000	-34.869056	-5.731161
C	0.000000	-33.821963	-5.089779
C	0.000000	-12.643038	7.698484
C	0.000000	-13.840231	7.064761
C	0.000000	-14.918781	6.478162
C	0.000000	-15.015868	-4.423542
C	0.000000	-13.985721	-5.073734
C	0.000000	-12.833551	-5.786630
C	0.000000	-11.784299	-6.419437
C	0.000000	-10.616574	-7.107185
C	0.000000	-9.562472	-7.718403
C	0.000000	-6.671034	9.288392
C	0.000000	-5.617433	8.676309
C	0.000000	-4.450185	7.987758
C	0.000000	-3.401189	7.354526
C	0.000000	-2.249311	6.641160
C	0.000000	-1.219150	5.990985
H	0.000000	33.357566	5.658952
B	0.000000	38.340795	-7.854950
C	0.000000	36.024770	-6.438418
C	0.000000	37.069533	-7.077765

C	0.738424	39.413230	-8.510149
C	-0.738424	39.413230	-8.510149
C	0.000000	33.821963	-5.089779
C	0.000000	34.869056	-5.731161
C	0.000000	40.501351	-9.174679
H	0.000000	40.539815	-10.264534
H	0.000000	41.488284	-8.711247
H	0.000000	-33.357566	5.658952
H	0.000000	-41.488284	-8.711247

**POM-17**

E= -7688.25733942

v= 0.3924

B	6.643561	34.894485	0.000000
B	-3.485497	40.531050	0.000000
C	-6.026626	40.343374	0.000000
C	7.822200	32.635296	0.000000
H	8.911620	32.551795	0.000000
C	-0.779143	40.692681	0.000000
C	-2.002712	40.631739	0.000000
C	5.948346	36.207828	0.000000
C	7.242206	33.785213	0.736519
C	7.242206	33.785213	-0.736519
C	-4.743539	40.456507	0.736638
C	-4.743539	40.456507	-0.736638
B	3.313693	40.829912	0.000000
C	1.801174	40.796181	0.000000
C	0.574232	40.751951	0.000000
C	5.355644	37.279996	0.000000
C	4.693072	38.461590	0.000000
C	4.083776	39.527436	0.000000
B	-9.392333	30.008494	0.000000
B	0.800780	24.403058	0.000000
B	-8.922599	17.970404	0.000000
C	3.360192	24.515979	0.000000
C	-10.562561	32.271320	0.000000
H	-11.651530	32.359712	0.000000
C	-9.918537	15.625487	0.000000
H	-10.997614	15.454385	0.000000
C	-7.810951	20.443292	0.000000
C	-8.327597	19.332527	0.000000
C	-1.905491	24.284763	0.000000
C	-0.681304	24.337858	0.000000
C	-8.695217	28.695403	0.000000
C	-9.141730	14.408701	0.000000
C	-8.484208	13.382843	0.000000
C	-7.745216	12.246852	0.000000
C	-9.432683	16.818257	0.736687
C	-9.432683	16.818257	-0.736687
C	-9.988435	31.118194	0.736807
C	-9.988435	31.118194	-0.736807
C	2.061551	24.458358	0.736301
C	2.061551	24.458358	-0.736301
B	8.023598	2.451582	0.000000
B	-2.211748	8.032665	0.000000
B	7.508035	14.467381	0.000000
C	-4.771295	7.922599	0.000000
C	9.221223	0.202988	0.000000
H	10.311170	0.127553	0.000000
C	8.505231	16.811671	0.000000
H	9.584423	16.982031	0.000000
C	6.396161	11.994486	0.000000
C	6.912601	13.105343	0.000000
C	0.494651	8.148503	0.000000
C	-0.729572	8.096168	0.000000
C	7.312603	3.756980	0.000000
C	6.333859	20.191510	0.000000
C	5.655729	21.212054	0.000000
C	4.893042	22.331893	0.000000
C	4.198477	23.332656	0.000000

C	8.018755	15.619126	0.736714	C	7.810951	-20.443292	0.000000
C	8.018755	15.619126	-0.736714	C	8.327597	-19.332527	0.000000
C	8.632482	1.348519	0.736676	C	1.905491	-24.284763	0.000000
C	8.632482	1.348519	-0.736676	C	0.681304	-24.337858	0.000000
C	-3.472593	7.978708	0.736300	C	8.695217	-28.695403	0.000000
C	-3.472593	7.978708	-0.736300	C	7.745216	-12.246852	0.000000
B	4.585858	8.323083	0.000000	C	7.066666	-11.226586	0.000000
B	-5.996839	24.112937	0.000000	C	6.303491	-10.107081	0.000000
C	-4.485063	24.174537	0.000000	C	5.608800	-9.106401	0.000000
C	-3.258381	24.226531	0.000000	C	9.432683	-16.818257	0.736687
C	-6.689339	22.769269	0.000000	C	9.432683	-16.818257	-0.736687
C	-7.229189	21.666577	0.000000	C	9.988435	-31.118194	0.736807
C	5.275866	9.667867	0.000000	C	9.988435	-31.118194	-0.736807
C	5.814851	10.771009	0.000000	C	-2.061551	-24.458358	0.736301
C	3.074244	8.258589	0.000000	C	-2.061551	-24.458358	-0.736301
C	1.847574	8.206246	0.000000	B	5.996839	-24.112937	0.000000
C	-7.066666	11.226586	0.000000	B	-4.585858	-8.323083	0.000000
C	7.072216	19.055104	0.000000	C	-3.074244	-8.258589	0.000000
C	7.729156	18.028873	0.000000	C	-1.847574	-8.206246	0.000000
C	-6.303491	10.107081	0.000000	C	-5.275866	-9.667867	0.000000
C	-5.608800	9.106401	0.000000	C	-5.814851	-10.771009	0.000000
C	6.702805	4.819458	0.000000	C	6.689339	-22.769269	0.000000
C	6.018982	5.988742	0.000000	C	7.229189	-21.666577	0.000000
C	5.387869	7.041881	0.000000	C	4.485063	-24.174537	0.000000
C	-8.094470	27.627780	0.000000	C	3.258381	-24.226531	0.000000
C	-7.419437	26.453427	0.000000	C	-5.655729	-21.212054	0.000000
C	-6.794709	25.396449	0.000000	C	8.484208	-13.382843	0.000000
C	4.090709	25.768562	0.000000	C	9.141730	-14.408701	0.000000
C	4.694211	26.826757	0.000000	C	-4.893042	-22.331893	0.000000
C	5.355700	28.009187	0.000000	C	-4.198477	-23.332656	0.000000
C	5.942412	29.084904	0.000000	C	8.094470	-27.627780	0.000000
C	6.580468	30.280503	0.000000	C	7.419437	-26.453427	0.000000
C	7.147707	31.358916	0.000000	C	6.794709	-25.396449	0.000000
C	-9.879707	33.543006	0.000000	C	-6.702805	-4.819458	0.000000
C	-9.300449	34.615054	0.000000	C	-6.018982	-5.988742	0.000000
C	-8.647928	35.803061	0.000000	C	-5.387869	-7.041881	0.000000
C	-8.047076	36.870961	0.000000	B	-6.643561	-34.894485	0.000000
C	-7.370637	38.045516	0.000000	B	3.485497	-40.531050	0.000000
C	-6.755489	39.097374	0.000000	C	6.026626	-40.343374	0.000000
B	-8.023598	-2.451582	0.000000	C	-7.822200	-32.635296	0.000000
B	2.211748	-8.032665	0.000000	H	-8.911620	-32.551795	0.000000
B	-7.508035	-14.467381	0.000000	C	0.779143	-40.692681	0.000000
C	4.771295	-7.922599	0.000000	C	2.002712	-40.631739	0.000000
C	-9.221223	-0.202988	0.000000	C	-5.948346	-36.207828	0.000000
H	-10.311170	-0.127553	0.000000	C	-7.242206	-33.785213	0.736519
C	-8.505231	-16.811671	0.000000	C	-7.242206	-33.785213	-0.736519
H	-9.584423	-16.982031	0.000000	C	4.743539	-40.456507	0.736638
C	-6.396161	-11.994486	0.000000	C	4.743539	-40.456507	-0.736638
C	-6.912601	-13.105343	0.000000	B	-3.313693	-40.829912	0.000000
C	-0.494651	-8.148503	0.000000	C	-1.801174	-40.796181	0.000000
C	0.729572	-8.096168	0.000000	C	-0.574232	-40.751951	0.000000
C	-7.312603	-3.756980	0.000000	C	-5.355644	-37.279996	0.000000
C	-7.729156	-18.028873	0.000000	C	-4.693072	-38.461590	0.000000
C	-7.072216	-19.055104	0.000000	C	-4.083776	-39.527436	0.000000
C	-6.333859	-20.191510	0.000000	C	6.755489	-39.097374	0.000000
C	-8.018755	-15.619126	0.736714	C	7.370637	-38.045516	0.000000
C	-8.018755	-15.619126	-0.736714	C	8.047076	-36.870961	0.000000
C	-8.632482	-1.348519	0.736676	C	8.647928	-35.803061	0.000000
C	-8.632482	-1.348519	-0.736676	C	9.300449	-34.615054	0.000000
C	3.472593	-7.978708	0.736300	C	9.879707	-33.543006	0.000000
C	3.472593	-7.978708	-0.736300	C	-7.147707	-31.358916	0.000000
B	9.392333	-30.008494	0.000000	C	-6.580468	-30.280503	0.000000
B	-0.800780	-24.403058	0.000000	C	-5.942412	-29.084904	0.000000
B	8.922599	-17.970404	0.000000	C	-5.355700	-28.009187	0.000000
C	-3.360192	-24.515979	0.000000	C	-4.694211	-26.826757	0.000000
C	10.562561	-32.271320	0.000000	C	-4.090709	-25.768562	0.000000
H	11.651530	-32.359712	0.000000	C	5.502880	-6.670513	0.000000
C	9.918537	-15.625487	0.000000	C	6.106978	-5.612673	0.000000
H	10.997614	-15.454385	0.000000	C	6.768579	-4.430311	0.000000

C	7.354614	-3.354236	0.000000
C	7.990329	-2.157399	0.000000
C	8.554618	-1.077447	0.000000
C	-8.554618	1.077447	0.000000
C	-7.990329	2.157399	0.000000
C	-7.354614	3.354236	0.000000
C	-6.768579	4.430311	0.000000
C	-6.106978	5.612673	0.000000
C	-5.502880	6.670513	0.000000
H	6.671049	-41.225711	0.000000
H	-6.671049	41.225711	0.000000
B	6.612191	46.785445	0.000000
C	5.298607	44.409532	0.000000
C	5.891569	45.481308	0.000000
C	7.219621	47.885668	0.738428
C	7.219621	47.885668	-0.738428
C	4.047060	42.150152	0.000000
C	4.642281	43.224163	0.000000
B	-6.612191	-46.785445	0.000000
C	-5.298607	-44.409532	0.000000
C	-5.891569	-45.481308	0.000000
C	-7.219621	-47.885668	0.738428
C	-7.219621	-47.885668	-0.738428
C	-4.047060	-42.150152	0.000000
C	-4.642281	-43.224163	0.000000
C	-7.835836	-49.001865	0.000000
H	-8.922970	-49.088037	0.000000
H	-7.329386	-49.967679	0.000000
C	7.835836	49.001865	0.000000
H	8.922970	49.088037	0.000000
H	7.329386	49.967679	0.000000

**POM-18**

E= -4974.00003776

v= 1.6153

B	-5.844192	-15.293367	0.000000
B	5.844192	-15.293367	0.000000
C	8.005391	-13.942750	0.000000
C	-8.005391	-13.942750	0.000000
H	-8.986493	-14.422139	0.000000
B	0.000000	-18.782149	0.000000
C	4.581096	-16.075954	0.000000
C	-4.581096	-16.075954	0.000000
C	-6.922212	-14.640047	0.736483
C	-6.922212	-14.640047	-0.736483
C	6.922212	-14.640047	0.736483
C	6.922212	-14.640047	-0.736483
B	5.890958	-3.401146	0.000000
B	-5.890958	-3.401146	0.000000
B	0.000000	6.802292	0.000000
C	-8.109212	-4.681856	0.000000
C	8.109212	-4.681856	0.000000
C	0.000000	9.363712	0.000000
B	0.000000	0.000000	0.000000
C	0.000000	1.511729	0.000000
C	-4.606001	-2.659276	0.000000
C	4.606001	-2.659276	0.000000
C	-4.515367	12.036196	0.000000
C	-5.710595	12.674910	0.000000
C	-6.791005	13.238368	0.000000
C	0.000000	8.063818	0.736582
C	0.000000	8.063818	-0.736582
C	6.983471	-4.031909	0.736582
C	6.983471	-4.031909	-0.736582
C	-6.983471	-4.031909	0.736582
C	-6.983471	-4.031909	-0.736582
B	-10.322349	12.707902	0.000000
B	-16.166540	2.585465	0.000000
C	-8.072080	13.904247	0.000000

H	-7.996692	14.993601	0.000000
C	-16.077471	0.038503	0.000000
H	-16.983185	-0.571462	0.000000
C	-16.265818	9.391074	0.000000
C	-16.261289	7.878017	0.000000
C	-11.631636	12.005322	0.000000
C	-14.860266	-0.738001	0.000000
C	-13.832091	-1.391934	0.000000
C	-12.681335	-2.107676	0.000000
C	-16.139759	1.325212	0.736483
C	-16.139759	1.325212	-0.736483
C	-9.217546	13.314835	0.736483
C	-9.217546	13.314835	-0.736483
B	10.322349	12.707902	0.000000
B	16.166540	2.585465	0.000000
C	8.072080	13.904247	0.000000
H	7.996692	14.993601	0.000000
C	16.077471	0.038503	0.000000
B	16.265818	9.391074	0.000000
C	16.261289	7.878017	0.000000
C	11.631636	12.005322	0.000000
C	16.139759	1.325212	0.736483
C	16.139759	1.325212	-0.736483
C	9.217546	13.314835	0.736483
C	9.217546	13.314835	-0.736483
C	8.069261	-12.500367	0.000000
C	8.121496	-11.282975	0.000000
C	8.165969	-9.928520	0.000000
C	-8.165969	-9.928520	0.000000
C	-8.121496	-11.282975	0.000000
C	-8.069261	-12.500367	0.000000
C	14.860266	-0.738001	0.000000
C	13.832091	-1.391934	0.000000
C	12.681335	-2.107676	0.000000
C	6.791005	13.238368	0.000000
C	5.710595	12.674910	0.000000
C	4.515367	12.036196	0.000000
H	8.986493	-14.422139	0.000000
H	16.983185	-0.571462	0.000000
C	-16.250960	6.650329	0.000000
C	-16.232950	5.295700	0.000000
C	-16.212732	4.070631	0.000000
C	0.000000	2.739453	0.000000
C	0.000000	4.093431	0.000000
C	0.000000	5.318552	0.000000
C	16.250960	6.650329	0.000000
C	16.232950	5.295700	0.000000
C	16.212732	4.070631	0.000000
C	-8.189734	-8.703219	0.000000
C	-8.189019	-7.348335	0.000000
C	-8.173149	-6.130250	0.000000
C	8.189734	-8.703219	0.000000
C	8.189019	-7.348335	0.000000
C	8.173149	-6.130250	0.000000
C	-12.702685	11.410297	0.000000
C	-13.884834	10.748580	0.000000
C	-14.953207	10.143681	0.000000
C	-3.545015	-2.046715	0.000000
C	-2.372436	-1.369727	0.000000
C	-1.309196	-0.755865	0.000000
C	3.530265	-16.705997	0.000000
C	2.366126	-17.398909	0.000000
C	1.308082	-18.021697	0.000000
C	-3.442342	11.444127	0.000000
C	-2.269335	10.766066	0.000000
C	-1.222378	10.143280	0.000000
C	-11.632076	-2.740908	0.000000
C	-10.458354	-3.417731	0.000000
C	-9.395527	-4.013030	0.000000

C	12.702685	11.410297	0.000000
C	13.884834	10.748580	0.000000
C	14.953207	10.143681	0.000000
C	3.545015	-2.046715	0.000000
C	2.372436	-1.369727	0.000000
C	1.309196	-0.755865	0.000000
C	-3.530265	-16.705997	0.000000
C	-2.366126	-17.398909	0.000000
C	-1.308082	-18.021697	0.000000
C	3.442342	11.444127	0.000000
C	2.269335	10.766066	0.000000
C	1.222378	10.143280	0.000000
C	11.632076	-2.740908	0.000000
C	10.458354	-3.417731	0.000000
C	9.395527	-4.013030	0.000000
B	22.161598	12.795005	0.000000
C	24.354177	14.060891	0.000000
H	24.418976	15.149480	0.000000
C	17.573586	10.146114	0.000000
C	23.249904	13.423338	-0.738467
C	23.249904	13.423338	0.738467
C	18.637016	10.760086	0.000000
C	19.810414	11.437548	0.000000
C	20.871181	12.049982	0.000000
B	0.000000	-25.590010	0.000000
C	0.000000	-28.121781	0.000000
H	-0.910346	-28.722194	0.000000
C	0.000000	-20.292229	0.000000
C	0.000000	-26.846676	0.738467
C	0.000000	-26.846676	-0.738467
C	0.000000	-21.520173	0.000000
C	0.000000	-22.875095	0.000000
C	0.000000	-24.099964	0.000000
B	-22.161598	12.795005	0.000000
C	-24.354177	14.060891	0.000000
H	-25.329323	13.572714	0.000000
C	-17.573586	10.146114	0.000000
C	-23.249904	13.423338	-0.738467
C	-23.249904	13.423338	0.738467
C	-18.637016	10.760086	0.000000
C	-19.810414	11.437548	0.000000
C	-20.871181	12.049982	0.000000
H	-24.418976	15.149480	0.000000
H	25.329323	13.572714	0.000000
H	0.910346	-28.722194	0.000000

**POM-19**

E= -761.729665232

v= 27.6593

B	0.000000	4.273338	0.000000
B	1.438401	3.442396	0.000000
B	-1.438401	3.442396	0.000000
C	3.592077	2.052377	0.000000
H	4.582374	2.512053	0.000000
C	-3.592077	2.052377	0.000000
H	-4.582374	2.512053	0.000000
B	0.000000	-4.273338	0.000000
B	1.438401	-3.442396	0.000000
B	-1.438401	-3.442396	0.000000
C	-3.592077	-2.052377	0.000000
H	-4.582374	-2.512053	0.000000
C	3.592077	-2.052377	0.000000
H	4.582374	-2.512053	0.000000
C	3.619162	0.604857	0.000000
C	3.619162	-0.604857	0.000000
C	-3.619162	0.604857	0.000000
C	-3.619162	-0.604857	0.000000
C	-2.517542	2.770505	0.729719
C	-2.517542	2.770505	-0.729719
C	-2.517542	-2.770505	0.729719

C	-2.517542	-2.770505	-0.729719
C	2.517542	-2.770505	0.729719
C	2.517542	-2.770505	-0.729719
C	2.517542	2.770505	0.729719
C	2.517542	2.770505	-0.729719
H	0.000000	5.468497	0.000000
H	0.000000	-5.468497	0.000000

**POM-20**

E= -1357.18762303

v= 13.4673

B	0.000000	0.000000	-2.204601
B	0.000000	0.000000	-0.545049
B	0.000000	1.458865	-2.992157
B	0.000000	-1.458865	-2.992157
C	0.000000	3.764079	-4.110331
H	0.000000	3.886637	-5.195153
C	0.000000	0.000000	2.029737
C	0.000000	-3.764079	-4.110331
H	0.000000	-3.886637	-5.195153
B	0.000000	-7.281358	2.251819
B	0.000000	-5.821584	3.044893
B	0.000000	-7.325504	0.591348
C	0.000000	-3.514492	4.161243
H	0.000000	-3.391262	5.246023
C	0.000000	-1.226423	2.810613
C	0.000000	-2.262687	3.433502
C	0.000000	-5.014014	-3.380216
C	0.000000	-6.046408	-2.749711
B	0.000000	7.281358	2.251819
B	0.000000	5.821584	3.044893
B	0.000000	7.325504	0.591348
C	0.000000	3.514492	4.161243
H	0.000000	3.391262	5.246023
C	0.000000	7.267029	-1.971115
H	0.000000	8.176223	-2.575468
C	0.000000	6.046408	-2.749711
C	0.000000	2.262687	3.433502
C	0.000000	1.226423	2.810613
C	0.000000	5.014014	-3.380216
C	-0.729727	7.317488	-0.679743
C	0.729727	7.317488	-0.679743
C	-0.729709	2.591379	-3.566760
C	0.729709	2.591379	-3.566760
C	-0.729655	4.685564	3.615710
C	0.729655	4.685564	3.615710
C	-0.729307	0.000000	0.726448
C	0.729307	0.000000	0.726448
C	-0.729655	-4.685564	3.615710
C	0.729655	-4.685564	3.615710
C	0.729709	-2.591379	-3.566760
C	-0.729709	-2.591379	-3.566760
C	0.729727	-7.317488	-0.679743
C	-0.729727	-7.317488	-0.679743
C	0.000000	-7.267029	-1.971115
H	0.000000	-8.176223	-2.575468
H	0.000000	-8.299989	2.876919
H	0.000000	8.299989	2.876919

**POM-21**

E= -1952.64550712

v= 6.7677

B	-2.206105	3.649010	0.000000
B	-0.546661	3.641424	0.000000
B	-2.986710	5.111640	0.000000
B	-3.002229	2.194681	0.000000
C	-4.093512	7.422171	0.000000
H	-5.177720	7.549978	0.000000

C	2.027991	3.629495	0.000000
C	-4.137398	-0.101940	0.000000
H	-5.222975	-0.217438	0.000000
B	2.206105	-3.649010	0.000000
B	3.002229	-2.194681	0.000000
B	0.546661	-3.641424	0.000000
B	2.986710	-5.111640	0.000000
C	-2.027991	-3.629495	0.000000
C	4.137398	0.101940	0.000000
H	5.222975	0.217438	0.000000
C	4.093512	-7.422171	0.000000
H	5.177720	-7.549978	0.000000
C	2.802124	2.398748	0.000000
C	3.418343	1.358524	0.000000
C	-3.418343	-1.358524	0.000000
C	-2.802124	-2.398748	0.000000
B	-2.285426	-10.909290	0.000000
B	-0.625190	-10.961237	0.000000
B	-3.071546	-9.445749	0.000000
C	1.937486	-10.914760	0.000000
H	2.537680	-11.826709	0.000000
C	-4.176796	-7.133323	0.000000
H	-5.260969	-7.004840	0.000000
C	-2.815109	-4.851791	0.000000
C	3.357224	-8.668431	0.000000
C	2.721728	-9.697754	0.000000
C	-3.443070	-5.884981	0.000000
B	2.285426	10.909290	0.000000
B	3.071546	9.445749	0.000000
B	0.625190	10.961237	0.000000
C	4.176796	7.133323	0.000000
H	5.260969	7.004840	0.000000
C	-1.937486	10.914760	0.000000
H	-2.537680	11.826709	0.000000
C	-2.721728	9.697754	0.000000
C	3.443070	5.884981	0.000000
C	2.815109	4.851791	0.000000
C	-3.357224	8.668431	0.000000
C	-0.645912	10.959300	0.729725
C	-0.645912	10.959300	-0.729725
C	-3.555731	6.246786	0.729746
C	-3.555731	6.246786	-0.729746
C	3.636767	8.306902	0.729644
C	3.636767	8.306902	-0.729644
C	0.724744	3.635539	0.729319
C	0.724744	3.635539	-0.729319
C	3.584006	-1.065602	0.729637
C	3.584006	-1.065602	-0.729637
C	-3.584006	1.065602	-0.729637
C	-3.584006	1.065602	0.729637
C	-3.636767	-8.306902	0.729644
C	-3.636767	-8.306902	-0.729644
C	-0.724744	-3.635539	-0.729319
C	-0.724744	-3.635539	0.729319
C	3.555731	-6.246786	0.729746
C	3.555731	-6.246786	-0.729746
C	0.645912	-10.959300	0.729725
C	0.645912	-10.959300	-0.729725
H	-2.915305	-11.924857	0.000000
H	2.915305	11.924857	0.000000

**POM-22**

E= -2548.10338019

v= 4.1604

B	0.000000	7.277058	2.213311
B	0.000000	7.277119	0.553865
B	0.000000	8.735817	3.001095
B	0.000000	5.818980	3.002638
C	0.000000	11.040876	4.119205

H	0.000000	11.163327	5.204024
C	0.000000	7.277205	-2.020804
C	0.000000	3.517084	4.127087
H	0.000000	3.396394	5.212097
B	0.000000	0.000000	-2.233507
B	0.000000	1.458046	-3.022885
B	0.000000	0.000000	-0.574150
B	0.000000	-1.458046	-3.022885
C	0.000000	0.000000	2.000424
C	0.000000	3.759866	-4.147132
H	0.000000	3.880438	-5.232148
C	0.000000	-3.759866	-4.147132
H	0.000000	-3.880438	-5.232148
C	0.000000	6.050131	-2.800767
C	0.000000	5.012928	-3.422046
C	0.000000	2.263890	3.402056
C	0.000000	1.226684	2.780783
B	0.000000	-7.277058	2.213311
B	0.000000	-7.277119	0.553865
B	0.000000	-8.735817	3.001095
B	0.000000	-5.818980	3.002638
C	0.000000	-11.040876	4.119205
H	0.000000	-11.163327	5.204024
C	0.000000	-7.277205	-2.020804
C	0.000000	-3.517084	4.127087
H	0.000000	-3.396394	5.212097
C	0.000000	-1.226684	2.780783
C	0.000000	-5.012928	-3.422046
C	0.000000	-6.050131	-2.800767
C	0.000000	-2.263890	3.402056
C	0.729753	-9.868159	3.575602
C	-0.729753	-9.868159	3.575602
B	0.000000	14.558036	-2.243170
B	0.000000	13.098217	-3.036260
B	0.000000	14.601988	-0.582665
C	0.000000	10.791246	-4.152870
H	0.000000	10.667999	-5.237640
C	0.000000	14.543657	1.979779
H	0.000000	15.452825	2.584157
C	0.000000	13.323015	2.758380
C	0.000000	9.539379	-3.425126
C	0.000000	8.503205	-2.802105
C	0.000000	12.290702	3.389009
C	0.729723	14.594056	0.688419
C	-0.729723	14.594056	0.688419
C	0.729753	9.868159	3.575602
C	-0.729753	9.868159	3.575602
C	0.729638	11.962159	-3.607098
C	-0.729638	11.962159	-3.607098
C	0.729319	7.277024	-0.717549
C	-0.729319	7.277024	-0.717549
C	0.729676	2.589687	-3.599298
C	-0.729676	2.589687	-3.599298
C	-0.729624	4.687133	3.579104
C	0.729624	4.687133	3.579104
C	0.729624	-4.687133	3.579104
C	-0.729624	-4.687133	3.579104
C	-0.729331	0.000000	0.697190
C	0.729331	0.000000	0.697190
C	0.729676	-2.589687	-3.599298
C	-0.729676	-2.589687	-3.599298
C	0.729319	-7.277024	-0.717549
C	-0.729319	-7.277024	-0.717549
B	0.000000	-14.558036	-2.243170
B	0.000000	-13.098217	-3.036260
B	0.000000	-14.601988	-0.582665
C	0.000000	-14.543657	1.979779
C	0.000000	-10.791246	-4.152870
H	0.000000	-10.667999	-5.237640

C	0.000000	-8.503205	-2.802105
C	0.000000	-9.539379	-3.425126
C	0.000000	-12.290702	3.389009
C	0.000000	-13.323015	2.758380
C	0.729638	-11.962159	-3.607098
C	-0.729638	-11.962159	-3.607098
C	-0.729723	-14.594056	0.688419
C	0.729723	-14.594056	0.688419
H	0.000000	-15.452825	2.584157
H	0.000000	-15.576709	-2.868258
H	0.000000	15.576709	-2.868258

**POM-23**

E= -3143.56125107

v= 2.7560

B	-2.228946	3.634742	0.000000
B	-0.569590	3.637165	0.000000
B	-3.020382	5.091671	0.000000
B	-3.016364	2.175613	0.000000
C	-4.147884	7.391865	0.000000
H	-5.233065	7.510911	0.000000
C	2.004954	3.641154	0.000000
C	-4.137567	-0.127701	0.000000
H	-5.222382	-0.249986	0.000000
B	2.228946	-3.634742	0.000000
B	3.016364	-2.175613	0.000000
B	0.569590	-3.637165	0.000000
B	3.020382	-5.091671	0.000000
C	-2.004954	-3.641154	0.000000
C	4.137567	0.127701	0.000000
H	5.222382	0.249986	0.000000
C	4.147884	-7.391865	0.000000
H	5.233065	-7.510911	0.000000
C	2.787354	2.415739	0.000000
C	3.410476	1.379649	0.000000
C	-3.410476	-1.379649	0.000000
C	-2.787354	-2.415739	0.000000
B	-2.207424	-10.918386	0.000000
B	-0.547951	-10.916027	0.000000
B	-2.992409	-12.378659	0.000000
B	-2.998917	-9.461514	0.000000
C	-4.106086	-14.685847	0.000000
H	-5.190686	-14.810267	0.000000
C	2.026698	-10.912327	0.000000
C	-4.126651	-7.161231	0.000000
H	-5.211817	-7.041981	0.000000
C	-2.783424	-4.869006	0.000000
C	3.424564	-8.645927	0.000000
C	2.804788	-9.684028	0.000000
C	-3.403272	-5.907062	0.000000
C	-3.564680	-13.512119	0.729757
C	-3.564680	-13.512119	-0.729757
B	2.207424	10.918386	0.000000
B	2.992409	12.378659	0.000000
B	2.998917	9.461514	0.000000
B	0.547951	10.916027	0.000000
C	4.126651	7.161231	0.000000
H	5.211817	7.041981	0.000000
C	4.106086	14.685847	0.000000
H	5.190686	14.810267	0.000000
C	-2.026698	10.912327	0.000000
C	-2.804788	9.684028	0.000000
C	3.403272	5.907062	0.000000
C	2.783424	4.869006	0.000000
C	-3.424564	8.645927	0.000000
C	3.564680	13.512119	-0.729757
C	3.564680	13.512119	0.729757
C	-0.723444	10.914119	0.729316
C	-0.723444	10.914119	-0.729316
C	-3.598401	6.222453	0.729685

C	-3.598401	6.222453	-0.729685
C	3.577050	8.330502	0.729621
C	3.577050	8.330502	-0.729621
C	0.701745	3.638956	0.729332
C	0.701745	3.638956	-0.729332
C	3.591356	-1.043188	0.729665
C	3.591356	-1.043188	-0.729665
C	-3.591356	1.043188	-0.729665
C	-3.591356	1.043188	0.729665
C	-3.577050	-8.330502	0.729621
C	-3.577050	-8.330502	-0.729621
C	-0.701745	-3.638956	-0.729332
C	-0.701745	-3.638956	0.729332
C	3.598401	-6.222453	0.729685
C	3.598401	-6.222453	-0.729685
C	0.723444	-10.914119	0.729316
C	0.723444	-10.914119	-0.729316
B	2.261947	-18.192814	0.000000
B	3.052635	-16.731737	0.000000
B	0.601565	-18.239670	0.000000
C	-1.960941	-18.185104	0.000000
C	4.164838	-14.422654	0.000000
H	5.249391	-14.297388	0.000000
C	2.810054	-12.137008	0.000000
C	3.434873	-13.172098	0.000000
C	-3.373701	-15.934382	0.000000
C	-2.741399	-16.965669	0.000000
C	3.621304	-15.594596	0.729641
C	3.621304	-15.594596	-0.729641
C	-0.669520	-18.233703	-0.729726
C	-0.669520	-18.233703	0.729726
H	-2.563997	-19.095167	0.000000
B	-2.261947	18.192814	0.000000
B	-0.601565	18.239670	0.000000
B	-3.052635	16.731737	0.000000
C	-4.164838	14.422654	0.000000
H	-5.249391	14.297388	0.000000
C	-3.621304	15.594596	0.729641
C	-3.621304	15.594596	-0.729641
C	0.669520	18.233703	0.729726
C	0.669520	18.233703	-0.729726
C	2.741399	16.965669	0.000000
C	3.373701	15.934382	0.000000
C	-3.434873	13.172098	0.000000
C	-2.810054	12.137008	0.000000
C	1.960941	18.185104	0.000000
H	2.563997	19.095167	0.000000
H	2.888686	-19.210309	0.000000
H	-2.888686	19.210309	0.000000

**POM-24**

E= -1812.98471046

v= 12.6159

B	0.000000	0.000000	0.000000
B	0.000000	1.656033	0.000000
B	-1.434167	-0.828017	0.000000
B	1.434167	-0.828017	0.000000
C	-3.662775	-2.114704	0.000000
C	0.000000	4.229408	0.000000
C	3.662775	-2.114704	0.000000
B	7.256363	4.189463	0.000000
B	5.825403	5.034126	0.000000
B	7.272383	2.527884	0.000000
C	3.572925	6.257804	0.000000
H	3.499929	7.347043	0.000000
C	1.232266	5.000593	0.000000
C	2.290296	5.585773	0.000000
C	4.946774	-1.433123	0.000000
C	5.982569	-0.809432	0.000000
B	-7.256363	4.189463	0.000000

B	-5.825403	5.034126	0.000000
B	-7.272383	2.527884	0.000000
C	-3.572925	6.257804	0.000000
H	-3.499929	7.347043	0.000000
C	-7.205879	-0.034658	0.000000
H	-8.112690	-0.642494	0.000000
C	-5.982569	-0.809432	0.000000
C	-2.290296	5.585773	0.000000
C	-1.232266	5.000593	0.000000
C	-4.946774	-1.433123	0.000000
C	-7.259034	1.256408	0.729645
C	-7.259034	1.256408	-0.729645
C	-2.534198	-1.463120	0.729703
C	-2.534198	-1.463120	-0.729703
C	-4.717598	5.658304	0.729645
C	-4.717598	5.658304	-0.729645
C	0.000000	2.926240	0.729703
C	0.000000	2.926240	-0.729703
C	4.717598	5.658304	0.729645
C	4.717598	5.658304	-0.729645
C	2.534198	-1.463120	-0.729703
C	2.534198	-1.463120	0.729703
C	7.259034	1.256408	-0.729645
C	7.259034	1.256408	0.729645
C	7.205879	-0.034658	0.000000
H	8.112690	-0.642494	0.000000
B	0.000000	-8.378926	0.000000
B	-1.446979	-7.562010	0.000000
B	1.446979	-7.562010	0.000000
C	3.632954	-6.223146	0.000000
C	-3.632954	-6.223146	0.000000
H	-4.612761	-6.704549	0.000000
C	-2.541436	-6.914711	-0.729645
C	-2.541436	-6.914711	0.729645
C	2.541436	-6.914711	0.729645
C	2.541436	-6.914711	-0.729645
C	-3.692274	-4.776341	0.000000
C	-3.714508	-3.567470	0.000000
C	3.692274	-4.776341	0.000000
C	3.714508	-3.567470	0.000000
H	4.612761	-6.704549	0.000000
H	8.291769	4.787255	0.000000
H	0.000000	-9.574510	0.000000
H	-8.291769	4.787255	0.000000

**POM-25**

E= -1218.79931015  
v= 11.1423

B	-4.729096	3.631369	0.000000
B	-4.729096	-3.631369	0.000000
C	-3.341961	5.768560	0.000000
H	-3.800496	6.759990	0.000000
C	-3.341961	-5.768560	0.000000
H	-3.800496	-6.759990	0.000000
B	-6.882103	0.000000	0.000000
C	-6.131988	-1.307684	0.000000
C	-5.517916	-2.368410	0.000000
C	-6.131988	1.307684	0.000000
C	-5.517916	2.368410	0.000000
C	-1.897654	-5.797896	0.000000
C	-0.681550	-5.812452	0.000000
C	0.681550	-5.812452	0.000000
C	1.897654	-5.797896	0.000000
C	-4.062072	-4.700132	0.735687
C	-4.062072	-4.700132	-0.735687
C	-4.062072	4.700132	0.735687
C	-4.062072	4.700132	-0.735687
B	4.729096	-3.631369	0.000000
B	4.729096	3.631369	0.000000

C	3.341961	-5.768560	0.000000
H	3.800496	-6.759990	0.000000
C	3.341961	5.768560	0.000000
H	3.800496	6.759990	0.000000
B	6.882103	0.000000	0.000000
C	6.131988	1.307684	0.000000
C	5.517916	2.368410	0.000000
C	6.131988	-1.307684	0.000000
C	5.517916	-2.368410	0.000000
C	1.897654	5.797896	0.000000
C	0.681550	5.812452	0.000000
C	-0.681550	5.812452	0.000000
C	-1.897654	5.797896	0.000000
C	4.062072	4.700132	0.735687
C	4.062072	4.700132	-0.735687
C	4.062072	-4.700132	0.735687
C	4.062072	-4.700132	-0.735687
H	-8.075122	0.000000	0.000000
H	8.075122	0.000000	0.000000

**POM-26**

E= -2195.12860135  
v= 4.9799

B	0.000000	8.015479	5.587055
B	0.000000	11.802040	-0.611989
C	0.000000	11.735122	-3.158908
C	0.000000	5.719756	6.692116
H	0.000000	5.595907	7.777414
B	0.000000	11.745131	3.609189
C	0.000000	11.786707	2.102330
C	0.000000	11.815725	0.877023
C	0.000000	10.423078	4.334025
C	0.000000	9.346141	4.919147
C	-0.735617	6.889548	6.152706
C	0.735617	6.889548	6.152706
C	-0.735722	11.791461	-1.871717
C	0.735722	11.791461	-1.871717
B	0.000000	3.734085	-5.550780
B	0.000000	0.000000	0.662584
B	0.000000	-3.734085	-5.550780
C	0.000000	0.000000	3.223235
C	0.000000	6.033294	-6.646311
H	0.000000	6.159582	-7.731309
C	0.000000	-6.033294	-6.646311
H	0.000000	-6.159582	-7.731309
B	0.000000	0.000000	-3.566409
C	0.000000	-1.319118	-4.311292
C	0.000000	-2.399484	-4.887335
C	0.000000	0.000000	-2.049454
C	0.000000	0.000000	-0.824968
C	0.000000	1.319118	-4.311292
C	0.000000	2.399484	-4.887335
C	0.000000	-7.280300	-5.917278
C	0.000000	-8.325414	-5.295347
C	0.000000	-9.488397	-4.584397
C	0.000000	-10.518348	-3.937649
C	-0.736303	-4.861356	-6.111470
C	0.736303	-4.861356	-6.111470
C	-0.736303	4.861356	-6.111470
C	0.736303	4.861356	-6.111470
C	-0.735850	0.000000	1.923666
C	0.735850	0.000000	1.923666
B	0.000000	-11.802040	-0.611989
B	0.000000	-8.015479	5.587055
C	0.000000	-11.735122	-3.158908
H	0.000000	-12.643708	-3.765111
C	0.000000	-5.719756	6.692116
H	0.000000	-5.595907	7.777414
B	0.000000	-11.745131	3.609189

C	0.000000	-10.423078	4.334025
C	0.000000	-9.346141	4.919147
C	0.000000	-11.786707	2.102330
C	0.000000	-11.815725	0.877023
C	0.000000	-4.469784	5.967671
C	0.000000	-3.421308	5.351563
C	0.000000	-2.254763	4.647229
C	0.000000	-1.221328	4.006927
C	-0.735617	-6.889548	6.152706
C	0.735617	-6.889548	6.152706
C	-0.735722	-11.791461	-1.871717
C	0.735722	-11.791461	-1.871717
C	0.000000	10.518348	-3.937649
C	0.000000	9.488397	-4.584397
C	0.000000	8.325414	-5.295347
C	0.000000	7.280300	-5.917278
C	0.000000	4.469784	5.967671
C	0.000000	3.421308	5.351563
C	0.000000	2.254763	4.647229
C	0.000000	1.221328	4.006927
H	0.000000	12.643708	-3.765111
H	0.000000	-12.763048	4.231436
H	0.000000	12.763048	4.231436

**POM-27**

E= -3171.45785401

v= 2.3232

B	0.574217	17.677689	0.000000
B	-5.613243	13.871088	0.000000
C	3.121342	17.618828	0.000000
H	3.724600	18.529447	0.000000
C	-6.710681	11.571703	0.000000
H	-7.795563	11.444234	0.000000
B	-3.646749	17.606741	0.000000
C	-4.367643	16.282508	0.000000
C	-4.949637	15.203893	0.000000
C	-2.140022	17.653152	0.000000
C	-0.914837	17.686485	0.000000
C	-5.982095	10.324102	0.000000
C	-5.362067	9.277942	0.000000
C	-4.653090	8.114218	0.000000
C	-4.009007	7.083136	0.000000
C	-6.175154	12.743265	0.735602
C	-6.175154	12.743265	-0.735602
C	1.833975	17.670959	0.735710
C	1.833975	17.670959	-0.735710
B	5.566557	2.159215	0.000000
B	-0.661087	5.872054	0.000000
B	5.540117	9.626016	0.000000
C	-3.221674	5.864205	0.000000
C	6.674317	-0.134131	0.000000
H	7.759933	-0.255101	0.000000
C	6.627946	11.928806	0.000000
H	7.712508	12.058774	0.000000
B	3.567817	5.885646	0.000000
C	4.308540	7.206977	0.000000
C	4.881074	8.289212	0.000000
C	2.050952	5.880464	0.000000
C	0.826474	5.876539	0.000000
C	4.317196	4.568822	0.000000
C	4.897199	3.490612	0.000000
C	5.894658	13.173321	0.000000
C	5.269048	14.216235	0.000000
C	4.554016	15.376711	0.000000
C	3.904059	16.404640	0.000000
C	6.097147	10.755065	0.736319
C	6.097147	10.755065	-0.736319
C	6.132477	1.034263	0.736203
C	6.132477	1.034263	-0.736203

C	-1.922126	5.867931	0.735859
C	-1.922126	5.867931	-0.735859
B	-5.566557	-2.159215	0.000000
B	0.661087	-5.872054	0.000000
B	-5.540117	-9.626016	0.000000
C	3.221674	-5.864205	0.000000
C	-6.674317	0.134131	0.000000
H	-7.759933	0.255101	0.000000
C	-6.627946	-11.928806	0.000000
H	-7.712508	-12.058774	0.000000
B	-3.567817	-5.885646	0.000000
C	-4.308540	-7.206977	0.000000
C	-4.881074	-8.289212	0.000000
C	-2.050952	-5.880464	0.000000
C	-0.826474	-5.876539	0.000000
C	-4.317196	-4.568822	0.000000
C	-4.897199	-3.490612	0.000000
C	-5.894658	-13.173321	0.000000
C	-5.269048	-14.216235	0.000000
C	-4.554016	-15.376711	0.000000
C	-3.904059	-16.404640	0.000000
C	-6.097147	-10.755065	0.736319
C	-6.097147	-10.755065	-0.736319
C	-6.132477	-1.034263	0.736203
C	-6.132477	-1.034263	-0.736203
C	1.922126	-5.867931	0.735859
C	1.922126	-5.867931	-0.735859
B	-0.574217	-17.677689	0.000000
B	5.613243	-13.871088	0.000000
C	-3.121342	-17.618828	0.000000
H	-3.724600	-18.529447	0.000000
C	6.710681	-11.571703	0.000000
H	7.795563	-11.444234	0.000000
B	3.646749	-17.606741	0.000000
C	4.367643	-16.282508	0.000000
C	4.949637	-15.203893	0.000000
C	2.140022	-17.653152	0.000000
C	0.914837	-17.686485	0.000000
C	5.982095	-10.324102	0.000000
C	5.362067	-9.277942	0.000000
C	4.653090	-8.114218	0.000000
C	4.009007	-7.083136	0.000000
C	6.175154	-12.743265	0.735602
C	6.175154	-12.743265	-0.735602
C	-1.833975	-17.670959	0.735710
C	-1.833975	-17.670959	-0.735710
C	-4.001660	4.640500	0.000000
C	-4.638773	3.605109	0.000000
C	-5.339333	2.436305	0.000000
C	-5.952189	1.385948	0.000000
C	5.952189	-1.385948	0.000000
C	5.339333	-2.436305	0.000000
C	4.638773	-3.605109	0.000000
C	4.001660	-4.640500	0.000000
H	4.271081	-18.623008	0.000000
H	-4.271081	18.623008	0.000000

**POM-28**

E= -4147.78710482

v= 1.4493

B	0.000000	3.732571	-5.582850
B	0.000000	0.000000	0.633095
B	0.000000	-3.732571	-5.582850
C	0.000000	0.000000	3.193638
C	0.000000	6.029394	-6.683248
H	0.000000	6.153623	-7.768494
C	0.000000	-6.029394	-6.683248
H	0.000000	-6.153623	-7.768494
B	0.000000	0.000000	-3.595748
C	0.000000	-1.319049	-4.340950



C	0.000000	-2.399044	-4.917633
C	0.000000	0.000000	-2.078967
C	0.000000	0.000000	-0.854488
C	0.000000	1.319049	-4.340950
C	0.000000	2.399044	-4.917633
C	0.000000	-7.278795	-5.958091
C	0.000000	-8.327242	-5.341978
C	0.000000	-9.493897	-4.637849
C	0.000000	-10.527532	-3.997895
C	-0.736215	-4.859288	-6.145105
C	0.736215	-4.859288	-6.145105
C	-0.736215	4.859288	-6.145105
C	0.736215	4.859288	-6.145105
C	-0.735869	0.000000	1.894100
C	0.735869	0.000000	1.894100
B	0.000000	-15.482811	5.559870
B	0.000000	-11.748876	-0.653699
B	0.000000	-8.016186	5.562077
C	0.000000	-11.748938	-3.214300
C	0.000000	-17.781910	6.655476
H	0.000000	-17.908025	7.740491
C	0.000000	-5.719414	6.662732
H	0.000000	-5.595146	7.747974
B	0.000000	-11.748986	3.575223
C	0.000000	-10.429713	4.320334
C	0.000000	-9.349660	4.896898
C	0.000000	-11.748706	2.058352
C	0.000000	-11.748674	0.833869
C	0.000000	-13.067909	4.320183
C	0.000000	-14.148240	4.896302
C	0.000000	-4.469916	5.937635
C	0.000000	-3.421428	5.321594
C	0.000000	-2.254854	4.617329
C	0.000000	-1.221290	3.977261
C	-0.736191	-6.889427	6.124441
C	0.736191	-6.889427	6.124441
C	-0.736323	-16.610064	6.120503
C	0.736323	-16.610064	6.120503
C	-0.735858	-11.748755	-1.914744
C	0.735858	-11.748755	-1.914744
B	0.000000	-19.764317	-5.578131
B	0.000000	-23.550667	0.621164
C	0.000000	-23.483711	3.168082
C	0.000000	-17.468610	-6.683259
H	0.000000	-17.344844	-7.768566
B	0.000000	-23.493815	-3.600000
C	0.000000	-23.535341	-2.093152
C	0.000000	-23.564373	-0.867848
C	0.000000	-22.171816	-4.324956
C	0.000000	-21.094942	-4.910186
C	-0.735604	-18.638311	-6.143686
C	0.735604	-18.638311	-6.143686
C	-0.735717	-23.539891	1.880892
C	0.735717	-23.539891	1.880892
C	0.000000	-12.970162	-3.998041
C	0.000000	-14.003598	-4.638341
C	0.000000	-15.170075	-5.342777
C	0.000000	-16.218520	-5.958932
C	0.000000	-19.029013	5.926609
C	0.000000	-20.074169	5.304751
C	0.000000	-21.237124	4.593761
C	0.000000	-22.267055	3.946984
B	0.000000	8.016186	5.562077
B	0.000000	15.482811	5.559870
B	0.000000	11.748876	-0.653699
C	0.000000	17.781910	6.655476
H	0.000000	17.908025	7.740491
C	0.000000	5.719414	6.662732
H	0.000000	5.595146	7.747974

C	0.000000	11.748938	-3.214300
B	0.000000	11.748986	3.575223
C	0.000000	11.748706	2.058352
C	0.000000	11.748674	0.833869
C	0.000000	13.067909	4.320183
C	0.000000	14.148240	4.896302
C	0.000000	10.429713	4.320334
C	0.000000	9.349660	4.896898
C	0.000000	12.970162	-3.998041
C	0.000000	14.003598	-4.638341
C	0.000000	15.170075	-5.342777
C	0.000000	16.218520	-5.958932
C	0.735858	11.748755	-1.914744
C	-0.735858	11.748755	-1.914744
C	0.736191	6.889427	6.124441
C	-0.736191	6.889427	6.124441
C	0.736323	16.610064	6.120503
C	-0.736323	16.610064	6.120503
B	0.000000	19.764317	-5.578131
B	0.000000	23.550667	0.621164
C	0.000000	17.468610	-6.683259
H	0.000000	17.344844	-7.768566
C	0.000000	23.483711	3.168082
H	0.000000	24.392527	3.774083
B	0.000000	23.493815	-3.600000
C	0.000000	23.535341	-2.093152
C	0.000000	23.564373	-0.867848
C	0.000000	22.171816	-4.324956
C	0.000000	21.094942	-4.910186
C	0.000000	22.267055	3.946984
C	0.000000	21.237124	4.593761
C	0.000000	20.074169	5.304751
C	0.000000	19.029013	5.926609
C	0.735717	23.539891	1.880892
C	-0.735717	23.539891	1.880892
C	0.735604	18.638311	-6.143686
C	-0.735604	18.638311	-6.143686
C	0.000000	1.221290	3.977261
C	0.000000	2.254854	4.617329
C	0.000000	3.421428	5.321594
C	0.000000	4.469916	5.937635
C	0.000000	7.278795	-5.958091
C	0.000000	8.327242	-5.341978
C	0.000000	9.493897	-4.637849
C	0.000000	10.527532	-3.997895
H	0.000000	-24.392527	3.774083
H	0.000000	-24.511694	-4.222172
H	0.000000	24.511694	-4.222172

**POM-29**

E= -5124.11635456  
v= 0.9359

B	-5.582379	9.601006	0.000000
B	0.637276	5.875025	0.000000
B	-5.574839	2.135807	0.000000
C	3.197821	5.877831	0.000000
C	-6.684930	11.896777	0.000000
H	-7.770278	12.020113	0.000000
C	-6.673001	-0.162081	0.000000
H	-7.758102	-0.287541	0.000000
B	-3.591561	5.870423	0.000000
C	-4.335415	4.550592	0.000000
C	-4.910985	3.470005	0.000000
C	-2.074786	5.872031	0.000000
C	-0.850306	5.873368	0.000000
C	-4.338158	7.188661	0.000000
C	-4.915912	8.268085	0.000000
C	-5.946447	-1.410713	0.000000
C	-5.329130	-2.458448	0.000000

C	-4.623754	-3.624347	0.000000	C	5.970774	-22.086235	0.000000
C	-3.982639	-4.657260	0.000000	C	5.353413	-21.038498	0.000000
C	-6.136041	1.008550	0.736211	C	4.647903	-19.872671	0.000000
C	-6.136041	1.008550	-0.736211	C	4.006515	-18.839910	0.000000
C	-6.145798	10.727122	0.736218	C	6.158183	-24.505803	0.735600
C	-6.145798	10.727122	-0.736218	C	6.158183	-24.505803	-0.735600
C	1.898280	5.876388	0.735870	C	-1.860786	-29.416107	0.735711
C	1.898280	5.876388	-0.735870	C	-1.860786	-29.416107	-0.735711
B	5.582379	-9.601006	0.000000	C	-3.980112	-7.099944	0.000000
B	-0.637276	-5.875025	0.000000	C	-4.619163	-8.134137	0.000000
B	5.574839	-2.135807	0.000000	C	-5.322072	-9.301526	0.000000
C	-3.197821	-5.877831	0.000000	C	-5.937220	-10.350537	0.000000
C	6.684930	-11.896777	0.000000	C	5.960859	-13.146751	0.000000
H	7.770278	-12.020113	0.000000	C	5.345631	-14.195717	0.000000
C	6.673001	0.162081	0.000000	C	4.642655	-15.363069	0.000000
H	7.758102	0.287541	0.000000	C	4.003628	-16.397275	0.000000
B	3.591561	-5.870423	0.000000	B	5.558625	13.896415	0.000000
C	4.335415	-4.550592	0.000000	B	5.548623	21.363271	0.000000
C	4.910985	-3.470005	0.000000	B	-0.660807	17.622405	0.000000
C	2.074786	-5.872031	0.000000	C	6.641636	23.663599	0.000000
C	0.850306	-5.873368	0.000000	H	7.726502	23.790981	0.000000
C	4.338158	-7.188661	0.000000	C	6.661315	11.600621	0.000000
C	4.915912	-8.268085	0.000000	H	7.746657	11.477228	0.000000
C	5.946447	1.410713	0.000000	C	-3.221406	17.619565	0.000000
C	5.329130	2.458448	0.000000	B	3.568115	17.627256	0.000000
C	4.623754	3.624347	0.000000	C	2.051243	17.625302	0.000000
C	3.982639	4.657260	0.000000	C	0.826760	17.623894	0.000000
C	6.136041	-1.008550	0.736211	C	4.311673	18.946961	0.000000
C	6.136041	-1.008550	-0.736211	C	4.886580	20.027938	0.000000
C	6.145798	-10.727122	0.736218	C	4.314640	16.308779	0.000000
C	6.145798	-10.727122	-0.736218	C	4.892247	15.229285	0.000000
C	-1.898280	-5.876388	0.735870	C	-4.006515	18.839910	0.000000
C	-1.898280	-5.876388	-0.735870	C	-4.647903	19.872671	0.000000
B	-5.558625	-13.896415	0.000000	C	-5.353413	21.038498	0.000000
B	0.660807	-17.622405	0.000000	C	-5.970774	22.086235	0.000000
B	-5.548623	-21.363271	0.000000	C	-1.921852	17.620843	-0.735858
C	3.221406	-17.619565	0.000000	C	-1.921852	17.620843	0.735858
C	-6.661315	-11.600621	0.000000	C	6.122069	12.770191	-0.736190
H	-7.746657	-11.477228	0.000000	C	6.122069	12.770191	0.736190
C	-6.641636	-23.663599	0.000000	C	6.108034	22.491127	-0.736322
H	-7.726502	-23.790981	0.000000	C	6.108034	22.491127	0.736322
B	-3.568115	-17.627256	0.000000	B	-5.594084	25.632544	0.000000
C	-4.311673	-18.946961	0.000000	B	0.601047	29.425804	0.000000
C	-4.886580	-20.027938	0.000000	C	-6.696486	23.335518	0.000000
C	-2.051243	-17.625302	0.000000	H	-7.781655	23.210554	0.000000
C	-0.826760	-17.623894	0.000000	C	3.148053	29.361595	0.000000
C	-4.314640	-16.308779	0.000000	H	3.753042	30.271061	0.000000
C	-4.892247	-15.229285	0.000000	B	-3.620076	29.364251	0.000000
C	-5.911306	-24.909845	0.000000	C	-2.113247	29.407430	0.000000
C	-5.288231	-25.954276	0.000000	C	-0.887984	29.437848	0.000000
C	-4.576180	-27.116581	0.000000	C	-4.343652	28.041461	0.000000
C	-3.928488	-28.145938	0.000000	C	-4.927688	26.963948	0.000000
C	-6.108034	-22.491127	0.736322	C	3.928488	28.145938	0.000000
C	-6.108034	-22.491127	-0.736322	C	4.576180	27.116581	0.000000
C	-6.122069	-12.770191	0.736190	C	5.288231	25.954276	0.000000
C	-6.122069	-12.770191	-0.736190	C	5.911306	24.909845	0.000000
C	1.921852	-17.620843	0.735858	C	1.860786	29.416107	-0.735711
C	1.921852	-17.620843	-0.735858	C	1.860786	29.416107	0.735711
B	-0.601047	-29.425804	0.000000	C	-6.158183	24.505803	-0.735600
B	5.594084	-25.632544	0.000000	C	-6.158183	24.505803	0.735600
C	-3.148053	-29.361595	0.000000	C	3.980112	7.099944	0.000000
H	-3.753042	-30.271061	0.000000	C	4.619163	8.134137	0.000000
C	6.696486	-23.335518	0.000000	C	5.322072	9.301526	0.000000
H	7.781655	-23.210554	0.000000	C	5.937220	10.350537	0.000000
B	3.620076	-29.364251	0.000000	C	-5.960859	13.146751	0.000000
C	4.343652	-28.041461	0.000000	C	-5.345631	14.195717	0.000000
C	4.927688	-26.963948	0.000000	C	-4.642655	15.363069	0.000000
C	2.113247	-29.407430	0.000000	C	-4.003628	16.397275	0.000000
C	0.887984	-29.437848	0.000000	H	4.243320	-30.381409	0.000000

H -4.243320 30.381409 0.000000

**POM-30**

E= -2955.61573784  
 v= 4.6916

B -3.655651 -11.419468 0.000000  
 B 3.655651 -11.419468 0.000000  
 C 5.823758 -10.080567 0.000000  
 C -5.823758 -10.080567 0.000000  
 H -6.804714 -10.561175 0.000000  
 B 0.000000 -13.531501 0.000000  
 C 1.310410 -12.785938 0.000000  
 C 2.378307 -12.184405 0.000000  
 C -1.310410 -12.785938 0.000000  
 C -2.378307 -12.184405 0.000000  
 C -4.738794 -10.775523 0.735573  
 C -4.738794 -10.775523 -0.735573  
 C 4.738794 -10.775523 0.735573  
 C 4.738794 -10.775523 -0.735573  
 B 3.660784 -2.113555 0.000000  
 B -3.660784 -2.113555 0.000000  
 B 0.000000 4.227110 0.000000  
 C -5.878128 -3.393739 0.000000  
 C 5.878128 -3.393739 0.000000  
 C 0.000000 6.787477 0.000000  
 B 0.000000 0.000000 0.000000  
 C 0.000000 1.515066 0.000000  
 C 0.000000 2.739428 0.000000  
 C -1.312085 -0.757533 0.000000  
 C -2.372414 -1.369714 0.000000  
 C 1.312085 -0.757533 0.000000  
 C 2.372414 -1.369714 0.000000  
 C -1.225326 7.564596 0.000000  
 C -2.276351 8.175597 0.000000  
 C -3.465457 8.841103 0.000000  
 C -4.537033 9.416102 0.000000  
 C 0.000000 5.487524 0.736063  
 C 0.000000 5.487524 -0.736063  
 C 4.752335 -2.743762 0.736063  
 C 4.752335 -2.743762 -0.736063  
 C -4.752335 -2.743762 0.736063  
 C -4.752335 -2.743762 -0.736063  
 B -8.061724 8.875621 0.000000  
 B -11.717375 2.543847 0.000000  
 C -5.818148 10.083806 0.000000  
 H -5.743889 11.173643 0.000000  
 C -11.641906 -0.003239 0.000000  
 H -12.548603 -0.612468 0.000000  
 B -11.718624 6.765751 0.000000  
 C -11.728152 5.258120 0.000000  
 C -11.741158 4.032528 0.000000  
 C -10.417742 7.527818 0.000000  
 C -9.362851 8.151877 0.000000  
 C -10.423100 -0.778865 0.000000  
 C -9.389348 -1.419378 0.000000  
 C -8.218451 -2.116421 0.000000  
 C -7.163795 -2.721135 0.000000  
 C -11.701274 1.283845 0.735573  
 C -11.701274 1.283845 -0.735573  
 C -6.962479 9.491678 0.735573  
 C -6.962479 9.491678 -0.735573  
 B 8.061724 8.875621 0.000000  
 B 11.717375 2.543847 0.000000  
 C 5.818148 10.083806 0.000000  
 H 5.743889 11.173643 0.000000  
 C 11.641906 -0.003239 0.000000  
 B 11.718624 6.765751 0.000000  
 C 11.728152 5.258120 0.000000  
 C 11.741158 4.032528 0.000000  
 C 10.417742 7.527818 0.000000

C 9.362851 8.151877 0.000000  
 C 11.701274 1.283845 0.735573  
 C 11.701274 1.283845 -0.735573  
 C 6.962479 9.491678 0.735573  
 C 6.962479 9.491678 -0.735573  
 C 5.886067 -8.637237 0.000000  
 C 5.923892 -7.421725 0.000000  
 C 5.942099 -6.059177 0.000000  
 C 5.938469 -4.843461 0.000000  
 C -5.938469 -4.843461 0.000000  
 C -5.942099 -6.059177 0.000000  
 C -5.923892 -7.421725 0.000000  
 C -5.886067 -8.637237 0.000000  
 C 10.423100 -0.778865 0.000000  
 C 9.389348 -1.419378 0.000000  
 C 8.218451 -2.116421 0.000000  
 C 7.163795 -2.721135 0.000000  
 C 4.537033 9.416102 0.000000  
 C 3.465457 8.841103 0.000000  
 C 2.276351 8.175597 0.000000  
 C 1.225326 7.564596 0.000000  
 H 6.804714 -10.561175 0.000000  
 H 12.548603 -0.612468 0.000000  
 H -12.751662 7.362175 0.000000  
 H 0.000000 -14.724351 0.000000  
 H 12.751662 7.362175 0.000000

**POM-31**

E= -1675.7565046  
 v= 5.5894

B 5.839340 6.022000 0.000000  
 B -5.839340 6.022000 0.000000  
 C 7.973362 4.629520 0.000000  
 H 8.964807 5.088557 0.000000  
 C -7.973362 4.629520 0.000000  
 H -8.964807 5.088557 0.000000  
 C -3.536553 7.452930 0.000000  
 C -4.586178 6.820483 0.000000  
 C 3.536553 7.452930 0.000000  
 C 4.586178 6.820483 0.000000  
 C -8.005120 3.186336 0.000000  
 C -8.027732 1.968005 0.000000  
 C -8.042763 0.612672 0.000000  
 C -6.905563 5.350249 0.736437  
 C -6.905563 5.350249 -0.736437  
 C 6.905563 5.350249 0.736437  
 C 6.905563 5.350249 -0.736437  
 B -5.839340 -6.022000 0.000000  
 B 5.839340 -6.022000 0.000000  
 C -7.973362 -4.629520 0.000000  
 H -8.964807 -5.088557 0.000000  
 C 7.973362 -4.629520 0.000000  
 H 8.964807 -5.088557 0.000000  
 C 3.536553 -7.452930 0.000000  
 C 4.586178 -6.820483 0.000000  
 C -3.536553 -7.452930 0.000000  
 C -4.586178 -6.820483 0.000000  
 C 8.042763 -0.612672 0.000000  
 C 8.042763 0.612672 0.000000  
 C 8.027732 1.968005 0.000000  
 C 8.005120 3.186336 0.000000  
 C 6.905563 -5.350249 0.736437  
 C 6.905563 -5.350249 -0.736437  
 C -6.905563 -5.350249 0.736437  
 C -6.905563 -5.350249 -0.736437  
 B 0.000000 -9.499636 0.000000  
 B 0.000000 9.499636 0.000000  
 C 1.304581 8.752630 0.000000  
 C 2.370913 8.141351 0.000000

C	-1.304581	8.752630	0.000000
C	-2.370913	8.141351	0.000000
C	1.304581	-8.752630	0.000000
C	2.370913	-8.141351	0.000000
C	-1.304581	-8.752630	0.000000
C	-2.370913	-8.141351	0.000000
C	-8.042763	-0.612672	0.000000
C	8.027732	-1.968005	0.000000
C	8.005120	-3.186336	0.000000
C	-8.027732	-1.968005	0.000000
C	-8.005120	-3.186336	0.000000
H	0.000000	10.693405	0.000000
H	0.000000	-10.693405	0.000000

**POM-32**

E= -3032.88295959

v= 2.5522

B	0.000000	10.221294	-8.139487
B	0.000000	16.299133	1.832576
C	0.000000	16.223092	4.379530
C	0.000000	7.922809	-9.239582
H	0.000000	7.799648	-10.325184
C	0.000000	16.321616	-0.878498
C	0.000000	16.327970	0.346919
C	0.000000	11.554883	-7.484502
C	0.736332	9.092949	-8.701117
C	-0.736332	9.092949	-8.701117
C	0.736470	16.281796	3.092614
C	-0.736470	16.281796	3.092614
B	0.000000	16.229924	-4.963471
C	0.000000	16.270436	-3.460790
C	0.000000	16.302910	-2.232101
C	0.000000	12.641431	-6.917845
C	0.000000	13.835979	-6.280928
C	0.000000	14.913042	-5.688811
B	0.000000	6.016500	8.105334
B	0.000000	0.000000	-1.875755
B	0.000000	-6.016500	8.105334
C	0.000000	0.000000	-4.437718
C	0.000000	8.317366	9.199034
H	0.000000	8.442157	10.284438
C	0.000000	-8.317366	9.199034
H	0.000000	-8.442157	10.284438
C	0.000000	-3.591943	6.891324
C	0.000000	-4.680271	7.453707
C	0.000000	0.000000	0.833107
C	0.000000	0.000000	-0.392242
C	0.000000	4.680271	7.453707
C	0.000000	-9.565578	8.474097
C	0.000000	-10.617621	7.859268
C	0.000000	-11.782910	7.166998
C	0.736775	-7.145715	8.663701
C	-0.736775	-7.145715	8.663701
C	0.736775	7.145715	8.663701
C	-0.736775	7.145715	8.663701
C	0.736312	0.000000	-3.137788
C	-0.736312	0.000000	-3.137788
B	0.000000	-16.299133	1.832576
B	0.000000	-10.221294	-8.139487
C	0.000000	-16.223092	4.379530
C	0.000000	-7.922809	-9.239582
H	0.000000	-7.799648	-10.325184
C	0.000000	-12.641431	-6.917845
C	0.000000	-11.554883	-7.484502
C	0.000000	-16.321616	-0.878498
C	0.000000	-16.327970	0.346919
C	0.000000	-4.450848	-7.218642
C	0.000000	-3.401550	-6.585898
C	0.000000	-2.249399	-5.872968

C	0.000000	-1.219126	-5.222960
C	0.736332	-9.092949	-8.701117
C	-0.736332	-9.092949	-8.701117
C	0.736470	-16.281796	3.092614
C	-0.736470	-16.281796	3.092614
B	0.000000	-16.229924	-4.963471
B	0.000000	0.000000	4.928170
C	0.000000	0.000000	3.415060
C	0.000000	0.000000	2.187276
C	0.000000	-1.314275	5.674542
C	0.000000	-2.393831	6.259371
C	0.000000	-14.913042	-5.688811
C	0.000000	-13.835979	-6.280928
C	0.000000	-16.270436	-3.460790
C	0.000000	-16.302910	-2.232101
C	0.000000	-12.829337	6.529492
C	0.000000	-5.618641	-7.906271
C	0.000000	-6.672668	-8.517644
C	0.000000	-13.979036	5.811632
C	0.000000	-15.007657	5.158358
C	0.000000	3.591943	6.891324
C	0.000000	2.393831	6.259371
C	0.000000	1.314275	5.674542
C	0.000000	1.219126	-5.222960
C	0.000000	2.249399	-5.872968
C	0.000000	3.401550	-6.585898
C	0.000000	4.450848	-7.218642
C	0.000000	5.618641	-7.906271
C	0.000000	6.672668	-8.517644
C	0.000000	9.565578	8.474097
C	0.000000	10.617621	7.859268
C	0.000000	11.782910	7.166998
C	0.000000	12.829337	6.529492
C	0.000000	13.979036	5.811632
C	0.000000	15.007657	5.158358
H	0.000000	17.249295	-5.584693
H	0.000000	17.131484	4.986544
H	0.000000	-17.249295	-5.584693
H	0.000000	-17.131484	4.986544

**POM-33**

E= -4390.00938548

v= 1.1191

B	-8.163181	-18.320192	0.000000
B	1.795703	-24.421232	0.000000
C	4.342843	-24.351072	0.000000
C	-9.258430	-16.019391	0.000000
H	-10.343766	-15.893924	0.000000
C	-0.915420	-24.437181	0.000000
C	0.309979	-24.446450	0.000000
C	-7.510890	-19.655092	0.000000
C	-8.722402	-17.190637	0.736342
C	-8.722402	-17.190637	-0.736342
C	3.055783	-24.406691	0.736439
C	3.055783	-24.406691	-0.736439
B	-5.000156	-24.335693	0.000000
C	-3.497583	-24.379805	0.000000
C	-2.268976	-24.415250	0.000000
C	-6.946392	-20.742763	0.000000
C	-6.312171	-21.938750	0.000000
C	-5.722475	-23.017138	0.000000
B	8.092968	-14.153619	0.000000
B	-1.875650	-8.114451	0.000000
B	8.120464	-2.122193	0.000000
C	-4.437593	-8.108126	0.000000
C	9.181338	-16.456972	0.000000
H	10.266450	-16.584281	0.000000
C	9.222212	0.174904	0.000000
H	10.308011	0.296280	0.000000

C	6.899578	-4.543067	0.000000
C	7.464789	-3.456211	0.000000
C	0.833211	-8.121055	0.000000
C	-0.392131	-8.118069	0.000000
C	7.444237	-12.815975	0.000000
C	8.502225	1.426117	0.000000
C	7.893101	2.481432	0.000000
C	7.207728	3.650547	0.000000
C	8.682307	-0.994418	0.736682
C	8.682307	-0.994418	-0.736682
C	8.648768	-15.284098	0.736793
C	8.648768	-15.284098	-0.736793
C	-3.137666	-8.111299	0.736290
C	-3.137666	-8.111299	-0.736290
B	-8.092968	14.153619	0.000000
B	1.875650	8.114451	0.000000
B	-8.120464	2.122193	0.000000
C	4.437593	8.108126	0.000000
C	-9.181338	16.456972	0.000000
H	-10.266450	16.584281	0.000000
C	-9.222212	-0.174904	0.000000
H	-10.308011	-0.296280	0.000000
C	-6.899578	4.543067	0.000000
C	-7.464789	3.456211	0.000000
C	-0.833211	8.121055	0.000000
C	0.392131	8.118069	0.000000
C	-7.444237	12.815975	0.000000
C	-7.207728	-3.650547	0.000000
C	-6.577319	-4.701270	0.000000
C	-5.867106	-5.855093	0.000000
C	-5.219733	-6.887017	0.000000
C	-8.682307	0.994418	0.736682
C	-8.682307	0.994418	-0.736682
C	-8.648768	15.284098	0.736793
C	-8.648768	15.284098	-0.736793
C	3.137666	8.111299	0.736290
C	3.137666	8.111299	-0.736290
B	-4.928206	8.130670	0.000000
B	4.928206	-8.130670	0.000000
C	3.415150	-8.127240	0.000000
C	2.187368	-8.124333	0.000000
C	5.677414	-6.817827	0.000000
C	6.264643	-5.739608	0.000000
C	-5.677414	6.817827	0.000000
C	-6.264643	5.739608	0.000000
C	-3.415150	8.127240	0.000000
C	-2.187368	8.124333	0.000000
C	6.577319	4.701270	0.000000
C	-7.893101	-2.481432	0.000000
C	-8.502225	-1.426117	0.000000
C	5.867106	5.855093	0.000000
C	5.219733	6.887017	0.000000
C	-6.884168	11.726449	0.000000
C	-6.254552	10.527118	0.000000
C	-5.671868	9.446395	0.000000
C	6.884168	-11.726449	0.000000
C	6.254552	-10.527118	0.000000
C	5.671868	-9.446395	0.000000
B	8.163181	18.320192	0.000000
B	-1.795703	24.421232	0.000000
C	-4.342843	24.351072	0.000000
C	9.258430	16.019391	0.000000
H	10.343766	15.893924	0.000000
C	0.915420	24.437181	0.000000
C	-0.309979	24.446450	0.000000
C	7.510890	19.655092	0.000000
C	8.722402	17.190637	0.736342
C	8.722402	17.190637	-0.736342
C	-3.055783	24.406691	0.736439

C	-3.055783	24.406691	-0.736439
B	5.000156	24.335693	0.000000
C	3.497583	24.379805	0.000000
C	2.268976	24.415250	0.000000
C	6.946392	20.742763	0.000000
C	6.312171	21.938750	0.000000
C	5.722475	23.017138	0.000000
C	-5.124639	23.137646	0.000000
C	-5.780479	22.110661	0.000000
C	-6.501103	20.962689	0.000000
C	-7.140924	19.917674	0.000000
C	-7.836121	18.754128	0.000000
C	-8.453403	17.703521	0.000000
C	8.533792	14.770723	0.000000
C	7.920050	13.718075	0.000000
C	7.229449	12.552037	0.000000
C	6.594046	11.504349	0.000000
C	5.878340	10.353920	0.000000
C	5.225866	9.325207	0.000000
C	-5.225866	-9.325207	0.000000
C	-5.878340	-10.353920	0.000000
C	-6.594046	-11.504349	0.000000
C	-7.229449	-12.552037	0.000000
C	-7.920050	-13.718075	0.000000
C	-8.533792	-14.770723	0.000000
C	8.453403	-17.703521	0.000000
C	7.836121	-18.754128	0.000000
C	7.140924	-19.917674	0.000000
C	6.501103	-20.962689	0.000000
C	5.780479	-22.110661	0.000000
C	5.124639	-23.137646	0.000000
H	-4.947685	25.261007	0.000000
H	5.623760	25.353582	0.000000
H	-5.623760	-25.353582	0.000000
H	4.947685	-25.261007	0.000000

**POM-34**

E= -5747.13580942

v= 0.6990

B	0.000000	32.536504	-1.840890
B	0.000000	26.457311	8.131334
C	0.000000	32.460370	-4.387857
C	0.000000	24.158857	9.231490
H	0.000000	24.035735	10.317100
C	0.000000	28.877046	6.908928
C	0.000000	27.790714	7.475986
C	0.000000	32.558524	0.870181
C	0.000000	32.565067	-0.355229
C	0.000000	22.908569	8.509701
C	0.000000	21.854504	7.898406
C	0.000000	20.686889	7.210479
C	0.736317	25.328926	8.692925
C	-0.736317	25.328926	8.692925
C	0.736419	32.519227	-3.100946
C	-0.736419	32.519227	-3.100946
B	0.000000	10.222206	-8.115983
B	0.000000	16.236714	1.867056
B	0.000000	22.253751	-8.114494
C	0.000000	16.236441	4.429031
C	0.000000	7.922566	-9.212379
H	0.000000	7.798629	-10.297894
C	0.000000	24.554814	-9.207640
H	0.000000	24.679830	-10.293023
C	0.000000	19.829234	-6.900389
C	0.000000	20.917534	-7.462808
C	0.000000	16.236790	-0.841803
C	0.000000	16.236758	0.383537
C	0.000000	11.557676	-7.463281
C	0.000000	28.020355	-7.175586
C	0.000000	29.066771	-6.538067

C	0.000000	30.216253	-5.819854	C	0.736261	-16.236484	3.129090
C	0.000000	31.244846	-5.166545	C	-0.736261	-16.236484	3.129090
C	0.736808	23.383091	-8.672591	B	0.000000	-16.237620	-4.936805
C	-0.736808	23.383091	-8.672591	B	0.000000	0.000000	4.955548
C	0.736690	9.093113	-8.675201	C	0.000000	0.000000	3.442550
C	-0.736690	9.093113	-8.675201	C	0.000000	0.000000	2.214768
C	0.736261	16.236484	3.129090	C	0.000000	-1.314325	5.702073
C	-0.736261	16.236484	3.129090	C	0.000000	-2.393718	6.287147
B	0.000000	16.237620	-4.936805	C	0.000000	-14.923152	-5.683207
B	0.000000	32.465861	4.955117	C	0.000000	-13.843687	-6.268128
C	0.000000	32.506721	3.452457	C	0.000000	-16.237434	-3.423746
C	0.000000	32.539503	2.223782	C	0.000000	-16.237203	-2.195965
C	0.000000	31.148853	5.680263	C	0.000000	-12.834790	6.576951
C	0.000000	30.071727	6.272248	C	0.000000	-5.618859	-7.878229
C	0.000000	17.551781	-5.683213	C	0.000000	-6.672896	-8.489554
C	0.000000	18.631284	-6.268145	C	0.000000	-13.986931	5.864016
C	0.000000	16.237434	-3.423746	C	0.000000	-15.017272	5.214135
C	0.000000	16.237203	-2.195965	C	0.000000	-19.829234	-6.900389
C	0.000000	19.637698	6.577567	C	0.000000	-18.631284	-6.268145
C	0.000000	26.855038	-7.867810	C	0.000000	-17.551781	-5.683213
C	0.000000	25.802947	-8.482552	C	0.000000	3.591571	6.919583
C	0.000000	18.485599	5.864559	C	0.000000	2.393718	6.287147
C	0.000000	17.455398	5.214444	C	0.000000	1.314325	5.702073
C	0.000000	12.645805	-6.900539	B	0.000000	-26.457311	8.131334
C	0.000000	13.843687	-6.268128	B	0.000000	-32.536504	-1.840890
C	0.000000	14.923152	-5.683207	C	0.000000	-32.460370	-4.387857
B	0.000000	6.014867	8.135523	C	0.000000	-24.158857	9.231490
B	0.000000	0.000000	-1.848249	H	0.000000	-24.035735	10.317100
B	0.000000	-6.014867	8.135523	C	0.000000	-32.558524	0.870181
C	0.000000	0.000000	-4.410197	C	0.000000	-32.565067	-0.355229
C	0.000000	8.314387	9.232045	C	0.000000	-27.790714	7.475986
H	0.000000	8.438312	10.317554	C	0.736317	-25.328926	8.692925
C	0.000000	-8.314387	9.232045	C	-0.736317	-25.328926	8.692925
H	0.000000	-8.438312	10.317554	C	0.736419	-32.519227	-3.100946
C	0.000000	-3.591571	6.919583	C	-0.736419	-32.519227	-3.100946
C	0.000000	-4.679549	7.482611	B	0.000000	-32.465861	4.955117
C	0.000000	0.000000	0.860616	C	0.000000	-32.506721	3.452457
C	0.000000	0.000000	-0.364720	C	0.000000	-32.539503	2.223782
C	0.000000	4.679549	7.482611	C	0.000000	-28.877046	6.908928
C	0.000000	-9.563999	8.509197	C	0.000000	-30.071727	6.272248
C	0.000000	-10.617867	7.897582	C	0.000000	-31.148853	5.680263
C	0.000000	-11.785485	7.209661	C	0.000000	-31.244846	-5.166545
C	0.736708	-7.143916	8.694898	C	0.000000	-30.216253	-5.819854
C	-0.736708	-7.143916	8.694898	C	0.000000	-29.066771	-6.538067
C	0.736708	7.143916	8.694898	C	0.000000	-28.020355	-7.175586
C	-0.736708	7.143916	8.694898	C	0.000000	-26.855038	-7.867810
C	0.736266	0.000000	-3.110262	C	0.000000	-25.802947	-8.482552
C	-0.736266	0.000000	-3.110262	C	0.000000	-22.908569	8.509701
B	0.000000	-22.253751	-8.114494	C	0.000000	-21.854504	7.898406
B	0.000000	-16.236714	1.867056	C	0.000000	-20.686889	7.210479
B	0.000000	-10.222206	-8.115983	C	0.000000	-19.637698	6.577567
C	0.000000	-16.236441	4.429031	C	0.000000	-18.485599	5.864559
C	0.000000	-24.554814	-9.207640	C	0.000000	-17.455398	5.214444
H	0.000000	-24.679830	-10.293023	C	0.000000	1.219084	-5.195397
C	0.000000	-7.922566	-9.212379	C	0.000000	2.249473	-5.845205
H	0.000000	-7.798629	-10.297894	C	0.000000	3.401643	-6.558095
C	0.000000	-12.645805	-6.900539	C	0.000000	4.450982	-7.190750
C	0.000000	-11.557676	-7.463281	C	0.000000	5.618859	-7.878229
C	0.000000	-16.236790	-0.841803	C	0.000000	6.672896	-8.489554
C	0.000000	-16.236758	0.383537	C	0.000000	9.563999	8.509197
C	0.000000	-20.917534	-7.462808	C	0.000000	10.617867	7.897582
C	0.000000	-4.450982	-7.190750	C	0.000000	11.785485	7.209661
C	0.000000	-3.401643	-6.558095	C	0.000000	12.834790	6.576951
C	0.000000	-2.249473	-5.845205	C	0.000000	13.986931	5.864016
C	0.000000	-1.219084	-5.195397	C	0.000000	15.017272	5.214135
C	0.736690	-9.093113	-8.675201	H	0.000000	-33.368568	-4.995017
C	-0.736690	-9.093113	-8.675201	H	0.000000	-33.485177	5.576623
C	0.736808	-23.383091	-8.672591	H	0.000000	33.368568	-4.995017
C	-0.736808	-23.383091	-8.672591	H	0.000000	33.485177	5.576623

**POM-35**

E= -7104.26218706

v= 0.4619

B	-8.146107	-34.565307	0.000000
B	1.825818	-40.649000	0.000000
C	4.372791	-40.574054	0.000000
C	-9.247530	-32.267472	0.000000
H	-10.333172	-32.144738	0.000000
C	-0.885274	-40.669562	0.000000
C	0.340142	-40.676817	0.000000
C	-7.490349	-35.898504	0.000000
C	-8.708472	-33.437326	0.736342
C	-8.708472	-33.437326	-0.736342
C	3.085856	-40.632107	0.736445
C	3.085856	-40.632107	-0.736445
B	-4.970159	-40.574048	0.000000
C	-3.467525	-40.616034	0.000000
C	-2.238864	-40.649739	0.000000
C	-6.923160	-36.984779	0.000000
C	-6.286354	-38.179397	0.000000
C	-5.694533	-39.256623	0.000000
B	8.102624	-30.370993	0.000000
B	-1.879162	-24.349609	0.000000
B	8.112397	-18.343935	0.000000
C	-4.441088	-24.347508	0.000000
C	9.197201	-32.671373	0.000000
H	10.282622	-32.795948	0.000000
C	9.213370	-16.046479	0.000000
H	10.299090	-15.924462	0.000000
C	6.892677	-20.765389	0.000000
C	7.457279	-19.678212	0.000000
C	0.829706	-24.351714	0.000000
C	-0.395642	-24.350752	0.000000
C	7.450420	-29.035033	0.000000
C	8.492487	-14.795779	0.000000
C	7.882013	-13.741244	0.000000
C	7.195125	-12.573020	0.000000
C	8.674031	-17.216054	0.736680
C	8.674031	-17.216054	-0.736680
C	8.661613	-31.499874	0.736799
C	8.661613	-31.499874	-0.736799
C	-3.141170	-24.348495	0.736290
C	-3.141170	-24.348495	-0.736290
B	-8.127765	-2.097897	0.000000
B	1.855631	-8.118169	0.000000
B	-8.136253	-14.123779	0.000000
C	4.417529	-8.120147	0.000000
C	-9.225395	0.201112	0.000000
H	-10.310937	0.324684	0.000000
C	-9.237082	-16.421243	0.000000
H	-10.322799	-16.543270	0.000000
C	-6.916486	-11.702292	0.000000
C	-7.481130	-12.789444	0.000000
C	-0.853244	-8.116098	0.000000
C	0.372100	-8.117023	0.000000
C	-7.474505	-3.433128	0.000000
C	-7.218628	-19.894562	0.000000
C	-6.586616	-20.944297	0.000000
C	-5.874551	-22.096977	0.000000
C	-5.225335	-23.127745	0.000000
C	-8.697833	-15.251614	0.736701
C	-8.697833	-15.251614	-0.736701
C	-8.687767	-0.969256	0.736693
C	-8.687767	-0.969256	-0.736693
C	3.117618	-8.119124	0.736296
C	3.117618	-8.119124	-0.736296
B	-4.948176	-8.113090	0.000000
B	4.924709	-24.354919	0.000000
C	3.411658	-24.353716	0.000000

C	2.183869	-24.352755	0.000000
C	5.672211	-23.041068	0.000000
C	6.258583	-21.962381	0.000000
C	-5.695829	-9.426717	0.000000
C	-6.282318	-10.505354	0.000000
C	-3.435188	-8.114174	0.000000
C	-2.207397	-8.115082	0.000000
C	6.563153	-11.523260	0.000000
C	-7.905579	-18.726372	0.000000
C	-8.516123	-17.671877	0.000000
C	5.851102	-10.370574	0.000000
C	5.201877	-9.339810	0.000000
C	-6.911386	-4.521071	0.000000
C	-6.278903	-5.718902	0.000000
C	-5.693944	-6.798367	0.000000
C	6.887663	-27.946897	0.000000
C	6.255411	-26.748951	0.000000
C	5.670484	-25.669434	0.000000
C	-5.227453	-25.565855	0.000000
C	-5.878414	-26.595530	0.000000
C	-6.592328	-27.747068	0.000000
C	-7.225871	-28.795888	0.000000
C	-7.914263	-29.963231	0.000000
C	-8.525935	-31.017086	0.000000
C	8.472340	-33.919616	0.000000
C	7.857017	-34.971375	0.000000
C	7.163892	-36.136154	0.000000
C	6.525580	-37.182097	0.000000
C	5.806554	-38.331066	0.000000
C	5.152382	-39.359119	0.000000
B	8.127765	2.097897	0.000000
B	-1.855631	8.118169	0.000000
B	8.136253	14.123779	0.000000
C	-4.417529	8.120147	0.000000
C	9.225395	-0.201112	0.000000
H	10.310937	-0.324684	0.000000
C	9.237082	16.421243	0.000000
H	10.322799	16.543270	0.000000
C	6.916486	11.702292	0.000000
C	7.481130	12.789444	0.000000
C	0.853244	8.116098	0.000000
C	-0.372100	8.117023	0.000000
C	7.474505	3.433128	0.000000
C	8.516123	17.671877	0.000000
C	7.905579	18.726372	0.000000
C	7.218628	19.894562	0.000000
C	8.697833	15.251614	0.736701
C	8.697833	15.251614	-0.736701
C	8.687767	0.969256	0.736693
C	8.687767	0.969256	-0.736693
C	-3.117618	8.119124	0.736296
C	-3.117618	8.119124	-0.736296
B	-8.102624	30.370993	0.000000
B	1.879162	24.349609	0.000000
B	-8.112397	18.343935	0.000000
C	4.441088	24.347508	0.000000
C	-9.197201	32.671373	0.000000
H	-10.282622	32.795948	0.000000
C	-9.213370	16.046479	0.000000
H	-10.299090	15.924462	0.000000
C	-6.892677	20.765389	0.000000
C	-7.457279	19.678212	0.000000
C	-0.829706	24.351714	0.000000
C	0.395642	24.350752	0.000000
C	-7.450420	29.035033	0.000000
C	-7.195125	12.573020	0.000000
C	-6.563153	11.523260	0.000000
C	-5.851102	10.370574	0.000000
C	-5.201877	9.339810	0.000000

C	-8.674031	17.216054	0.736680
C	-8.674031	17.216054	-0.736680
C	-8.661613	31.499874	0.736799
C	-8.661613	31.499874	-0.736799
C	3.141170	24.348495	0.736290
C	3.141170	24.348495	-0.736290
B	-4.924709	24.354919	0.000000
B	4.948176	8.113090	0.000000
C	3.435188	8.114174	0.000000
C	2.207397	8.115082	0.000000
C	5.695829	9.426717	0.000000
C	6.282318	10.505354	0.000000
C	-5.672211	23.041068	0.000000
C	-6.258583	21.962381	0.000000
C	-3.411658	24.353716	0.000000
C	-2.183869	24.352755	0.000000
C	6.586616	20.944297	0.000000
C	-7.882013	13.741244	0.000000
C	-8.492487	14.795779	0.000000
C	5.874551	22.096977	0.000000
C	5.225335	23.127745	0.000000
C	-6.887663	27.946897	0.000000
C	-6.255411	26.748951	0.000000
C	-5.670484	25.669434	0.000000
C	6.911386	4.521071	0.000000
C	6.278903	5.718902	0.000000
C	5.693944	6.798367	0.000000
B	8.146107	34.565307	0.000000
B	-1.825818	40.649000	0.000000
C	-4.372791	40.574054	0.000000
C	9.247530	32.267472	0.000000
H	10.333172	32.144738	0.000000
C	0.885274	40.669562	0.000000
C	-0.340142	40.676817	0.000000
C	7.490349	35.898504	0.000000
C	8.708472	33.437326	0.736342
C	8.708472	33.437326	-0.736342
C	-3.085856	40.632107	0.736445
C	-3.085856	40.632107	-0.736445
B	4.970159	40.574048	0.000000
C	3.467525	40.616034	0.000000
C	2.238864	40.649739	0.000000
C	6.923160	36.984779	0.000000
C	6.286354	38.179397	0.000000
C	5.694533	39.256623	0.000000
C	-5.152382	39.359119	0.000000
C	-5.806554	38.331066	0.000000
C	-6.525580	37.182097	0.000000
C	-7.163892	36.136154	0.000000
C	-7.857017	34.971375	0.000000
C	-8.472340	33.919616	0.000000
C	8.525935	31.017086	0.000000
C	7.914263	29.963231	0.000000
C	7.225871	28.795888	0.000000
C	6.592328	27.747068	0.000000
C	5.878414	26.595530	0.000000
C	5.227453	25.565855	0.000000
C	-5.203748	6.901680	0.000000
C	-5.854556	5.871916	0.000000
C	-6.568374	4.720324	0.000000
C	-7.201949	3.671531	0.000000
C	-7.890606	2.504349	0.000000
C	-8.502671	1.450737	0.000000
C	8.502671	-1.450737	0.000000
C	7.890606	-2.504349	0.000000
C	7.201949	-3.671531	0.000000
C	6.568374	-4.720324	0.000000
C	5.854556	-5.871916	0.000000
C	5.203748	-6.901680	0.000000

H	-4.979402	41.482728	0.000000
H	5.592272	41.592865	0.000000
H	-5.592272	-41.592865	0.000000
H	4.979402	-41.482728	0.000000

**POM-36**

E= -4098.00746873

v= 2.3126

B	-5.880136	-15.290400	0.000000
B	5.880136	-15.290400	0.000000
C	8.043261	-13.943386	0.000000
C	-8.043261	-13.943386	0.000000
H	-9.025042	-14.422697	0.000000
B	0.000000	-18.699509	0.000000
C	4.611955	-16.064617	0.000000
C	-4.611955	-16.064617	0.000000
C	-6.960291	-14.640851	0.736331
C	-6.960291	-14.640851	-0.736331
C	6.960291	-14.640851	0.736331
C	6.960291	-14.640851	-0.736331
B	5.891123	-3.401242	0.000000
B	-5.891123	-3.401242	0.000000
B	0.000000	6.802483	0.000000
C	-8.109569	-4.682062	0.000000
C	8.109569	-4.682062	0.000000
C	0.000000	9.364123	0.000000
B	0.000000	0.000000	0.000000
C	0.000000	1.511766	0.000000
C	-4.606224	-2.659404	0.000000
C	4.606224	-2.659404	0.000000
C	-4.504392	12.055555	0.000000
C	-5.696377	12.700330	0.000000
C	-6.773656	13.269733	0.000000
C	0.000000	8.064064	0.736429
C	0.000000	8.064064	-0.736429
C	6.983684	-4.032032	0.736429
C	6.983684	-4.032032	-0.736429
C	-6.983684	-4.032032	0.736429
C	-6.983684	-4.032032	-0.736429
B	-10.301807	12.737547	0.000000
B	-16.181943	2.552853	0.000000
C	-8.053696	13.937362	0.000000
H	-7.977901	15.027264	0.000000
C	-16.096957	0.006024	0.000000
H	-17.002943	-0.604567	0.000000
B	-16.194250	9.349755	0.000000
C	-16.203492	7.846482	0.000000
C	-11.606389	12.026379	0.000000
C	-14.878754	-0.768708	0.000000
C	-13.846997	-1.416958	0.000000
C	-12.692613	-2.126860	0.000000
C	-16.159495	1.292636	0.736331
C	-16.159495	1.292636	-0.736331
C	-9.199203	13.348215	0.736331
C	-9.199203	13.348215	-0.736331
B	10.301807	12.737547	0.000000
B	16.181943	2.552853	0.000000
C	8.053696	13.937362	0.000000
H	7.977901	15.027264	0.000000
C	16.096957	0.006024	0.000000
B	16.194250	9.349755	0.000000
C	16.203492	7.846482	0.000000
C	11.606389	12.026379	0.000000
C	16.159495	1.292636	0.736331
C	16.159495	1.292636	-0.736331
C	9.199203	13.348215	0.736331
C	9.199203	13.348215	-0.736331
C	8.105098	-12.501025	0.000000
C	8.150620	-11.283372	0.000000



C	8.188221	-9.928695	0.000000
C	-8.188221	-9.928695	0.000000
C	-8.150620	-11.283372	0.000000
C	-8.105098	-12.501025	0.000000
C	14.878754	-0.768708	0.000000
C	13.846997	-1.416958	0.000000
C	12.692613	-2.126860	0.000000
C	6.773656	13.269733	0.000000
C	5.696377	12.700330	0.000000
C	4.504392	12.055555	0.000000
H	9.025042	-14.422697	0.000000
H	17.002943	-0.604567	0.000000
H	-17.228151	9.946678	0.000000
H	0.000000	-19.893355	0.000000
H	17.228151	9.946678	0.000000
C	-16.218866	6.617466	0.000000
C	-16.222669	5.263685	0.000000
C	-16.218344	4.038238	0.000000
C	0.000000	2.739524	0.000000
C	0.000000	4.093539	0.000000
C	0.000000	5.318809	0.000000
C	16.218866	6.617466	0.000000
C	16.222669	5.263685	0.000000
C	16.218344	4.038238	0.000000
C	-8.203688	-8.703475	0.000000
C	-8.196472	-7.348599	0.000000
C	-8.174711	-6.130617	0.000000
C	8.203688	-8.703475	0.000000
C	8.196472	-7.348599	0.000000
C	8.174711	-6.130617	0.000000
C	-12.669820	11.417401	0.000000
C	-13.840327	10.737217	0.000000
C	-14.896999	10.109394	0.000000
C	-3.545109	-2.046769	0.000000
C	-2.372497	-1.369762	0.000000
C	-1.309228	-0.755883	0.000000
C	3.552849	-16.681086	0.000000
C	2.378540	-17.354683	0.000000
C	1.306493	-17.955877	0.000000
C	-3.435586	11.456340	0.000000
C	-2.265838	10.772653	0.000000
C	-1.221915	10.144816	0.000000
C	-11.639274	-2.752865	0.000000
C	-10.462310	-3.424053	0.000000
C	-9.396626	-4.014199	0.000000
C	12.669820	11.417401	0.000000
C	13.840327	10.737217	0.000000
C	14.896999	10.109394	0.000000
C	3.545109	-2.046769	0.000000
C	2.372497	-1.369762	0.000000
C	1.309228	-0.755883	0.000000
C	-3.552849	-16.681086	0.000000
C	-2.378540	-17.354683	0.000000
C	-1.306493	-17.955877	0.000000
C	3.435586	11.456340	0.000000
C	2.265838	10.772653	0.000000
C	1.221915	10.144816	0.000000
C	11.639274	-2.752865	0.000000
C	10.462310	-3.424053	0.000000
C	9.396626	-4.014199	0.000000

**C1**

E= -3177.96236744

v= 3.7856

B	0.358497	-5.485616	-5.914853
B	5.875534	-5.555048	-1.196814
C	-2.162747	-5.531699	-6.275028
H	-2.608352	-5.539047	-7.272513
C	6.595916	-5.564289	1.281226

H	7.644861	-5.546011	1.581177
B	4.513454	-5.424764	-5.183952
C	5.020984	-5.469278	-3.761646
C	5.430534	-5.506801	-2.606815
C	3.034724	-5.443016	-5.461818
C	1.829485	-5.461263	-5.685009
C	5.655494	-5.570024	2.370536
C	4.859906	-5.565129	3.290820
C	3.955664	-5.557392	4.309300
C	3.136354	-5.548211	5.207873
C	6.272917	-6.200387	0.014536
C	-0.871529	-6.245765	-6.112182
B	-0.358512	-5.485539	5.914857
B	-5.875550	-5.555014	1.196818
C	2.162731	-5.531626	6.275034
H	2.608335	-5.538964	7.272519
C	-6.595933	-5.564289	-1.281221
H	-7.644878	-5.546017	-1.581173
B	-4.513470	-5.424681	5.183955
C	-5.020999	-5.469211	3.761649
C	-5.430550	-5.506748	2.606819
C	-3.034739	-5.442934	5.461821
C	-1.829500	-5.461184	5.685012
C	-5.655511	-5.570036	-2.370531
C	-4.859922	-5.565154	-3.290814
C	-3.955679	-5.557435	-4.309294
C	-3.136369	-5.548271	-5.207867
C	-6.272932	-6.200370	-0.014522
C	0.871511	-6.245690	6.112194
B	0.358532	5.485607	-5.914852
B	5.875559	5.555035	-1.196806
C	-2.162712	5.531691	-6.275028
H	-2.608316	5.539035	-7.272513
C	6.595932	5.564273	1.281236
H	7.644876	5.545991	1.581192
B	4.513489	5.424755	-5.183948
C	5.021017	5.469268	-3.761641
C	5.430564	5.506790	-2.606809
C	3.034759	5.443006	-5.461816
C	1.829519	5.461253	-5.685008
C	5.655505	5.570010	2.370542
C	4.859911	5.565119	3.290820
C	3.955665	5.557385	4.309297
C	3.136352	5.548206	5.207868
C	6.272941	6.200372	0.014545
C	-0.871494	6.245756	-6.112183
B	-0.358514	5.485541	5.914851
B	-5.875542	5.555032	1.196806
C	2.162729	5.531619	6.275028
H	2.608333	5.538954	7.272513
C	-6.595916	5.564303	-1.281236
H	-7.644860	5.546034	-1.581192
B	-4.513472	5.424699	5.183946
C	-5.020999	5.469231	3.761639
C	-5.430547	5.506769	2.606808
C	-3.034741	5.442946	5.461814
C	-1.829502	5.461190	5.685006
C	-5.655489	5.570048	-2.370542
C	-4.859895	5.565163	-3.290820
C	-3.955648	5.557439	-4.309297
C	-3.136335	5.548268	-5.207868
C	-6.272920	6.200387	-0.014537
C	0.871511	6.245687	6.112190
C	6.269742	-4.734825	0.023663
C	0.898568	-4.775107	6.113057
C	-6.269761	-4.734808	-0.023670
C	-0.898581	-4.775182	-6.113061
C	-0.898548	4.775173	-6.113056
C	6.269762	4.734810	0.023671

C	-6.269751	4.734825	-0.023682
C	0.898564	4.775104	6.113049
C	6.337862	-0.620792	-0.217437
C	-6.337863	-0.620776	0.217436
C	-6.337862	0.620793	0.217434
C	6.337864	0.620777	-0.217435
H	-5.293666	-5.384776	6.084775
H	-5.293669	5.384798	6.084765
H	5.293686	5.384862	-6.084768
H	5.293651	-5.384874	-6.084773
Ag	-6.280765	-2.628914	0.145248
Ag	-6.280760	2.628932	0.145240
Ag	6.280768	2.628916	-0.145245
Ag	6.280755	-2.628930	-0.145251

**C2**

E= -5137.15103626

v= 2.4447

B	-0.124428	3.621901	4.731550
B	0.124414	-3.621922	4.731554
C	-0.100818	5.790628	3.334562
H	-0.101127	6.778035	3.799006
C	0.100806	-5.790650	3.334568
H	0.101112	-6.778057	3.799013
B	-0.000009	-0.000009	6.881005
C	0.050741	-1.305551	6.127292
C	0.086145	-2.365410	5.512406
C	-0.050758	1.305532	6.127291
C	-0.086161	2.365390	5.512404
C	0.063030	-5.802469	1.895791
C	0.022830	-5.817620	0.680330
C	-0.022826	-5.817619	-0.680283
C	-0.063026	-5.802468	-1.895744
C	0.752842	-4.711067	4.055458
C	0.712474	4.719577	4.087923
B	-0.124415	-3.621926	-4.731511
B	0.124426	3.621894	-4.731515
C	-0.100805	-5.790652	-3.334522
H	-0.101113	-6.778060	-3.798965
C	0.100817	5.790621	-3.334528
H	0.101130	6.778029	-3.798972
B	0.000009	-0.000017	-6.880968
C	0.050757	1.305524	-6.127256
C	0.086160	2.365383	-5.512369
C	-0.050743	-1.305557	-6.127255
C	-0.086147	-2.365416	-5.512367
C	0.063032	5.802439	-1.895750
C	0.022827	5.817592	-0.680289
C	-0.022833	5.817594	0.680324
C	-0.063037	5.802445	1.895785
C	0.752855	4.711037	-4.055414
C	0.712487	-4.719601	-4.087883
B	-10.958056	3.682422	4.647714
B	-11.001515	-3.575193	4.808998
C	-11.014813	5.800495	3.233739
H	-11.032839	6.797901	3.679194
C	-11.009410	-5.765351	3.443854
H	-10.983171	-6.746452	3.920663
B	-10.879151	0.098463	6.872731
C	-10.919560	-1.227945	6.150514
C	-10.954844	-2.303052	5.562579
C	-10.903596	1.386004	6.094290
C	-10.927189	2.433086	5.457263
C	-11.024284	-5.792488	2.005099
C	-11.026592	-5.815234	0.788805
C	-11.026606	-5.822590	-0.573166
C	-11.024032	-5.813026	-1.789181
C	-11.645431	-4.682403	4.175666
C	-11.723139	4.724117	3.970400
B	-10.958055	-3.682410	-4.647740

B	-11.001500	3.575205	-4.809024
C	-11.014822	-5.800483	-3.233765
H	-11.032853	-6.797889	-3.679220
C	-11.009398	5.765363	-3.443880
H	-10.983158	6.746464	-3.920689
B	-10.879135	-0.098452	-6.872757
C	-10.919544	1.227957	-6.150540
C	-10.954828	2.303064	-5.562605
C	-10.903585	-1.385992	-6.094316
C	-10.927182	-2.433075	-5.457289
C	-11.024275	5.792500	-2.005125
C	-11.026584	5.815246	-0.788831
C	-11.026598	5.822602	0.573140
C	-11.024024	5.813038	1.789154
C	-11.645418	4.682415	-4.175694
C	-11.723143	-4.724101	-3.970426
C	-0.712487	-4.719597	4.087925
C	-0.752843	-4.711070	-4.055412
C	-0.712475	4.719572	-4.087890
C	-0.752855	4.711045	4.055451
C	-10.252731	4.757149	3.960463
C	-10.180077	-4.678731	4.156973
C	-10.180064	4.678743	-4.156997
C	-10.252736	-4.757141	-3.960490
C	-4.822575	-4.572734	4.346499
C	-4.822561	4.572725	-4.346496
C	-6.064105	4.563990	-4.350322
C	-6.064118	-4.563992	4.350316
H	0.000011	-0.000018	-8.072506
H	-10.837362	-0.117281	-8.064219
H	-10.837383	0.117292	8.064193
H	-0.000011	-0.000009	8.072543
Ag	-2.815216	4.600812	-4.248678
Ag	-8.073155	4.569343	-4.273221
Ag	-8.073168	-4.569337	4.273205
Ag	-2.815229	-4.600829	4.248696
B	11.001510	3.575212	4.808998
B	10.958096	-3.682403	4.647711
C	11.009387	5.765370	3.443855
H	10.983143	6.746471	3.920665
C	11.014860	-5.800475	3.233734
H	11.032896	-6.797881	3.679188
B	10.879178	-0.098447	6.872730
C	10.903628	-1.385987	6.094289
C	10.927223	-2.433068	5.457260
C	10.919575	1.227963	6.150514
C	10.954849	2.303070	5.562579
C	11.024066	-5.813017	1.789149
C	11.026635	-5.822580	0.573135
C	11.026617	-5.815225	-0.788836
C	11.024303	-5.792478	-2.005130
C	10.252775	-4.757135	3.960462
B	11.001506	-3.575182	-4.809029
B	10.958019	3.682432	-4.647740
C	11.009419	-5.765340	-3.443885
H	10.983182	-6.746442	-3.920695
C	11.014777	5.800504	-3.233764
H	11.032798	6.797911	-3.679218
B	10.879113	0.098475	-6.872759
C	10.903559	1.386015	-6.094318
C	10.927151	2.433097	-5.457290
C	10.919532	-1.227934	-6.150544
C	10.954824	-2.303041	-5.562609
C	11.023994	5.813046	-1.789179
C	11.026571	5.822610	-0.573165
C	11.026562	5.815254	0.788806
C	11.024258	5.792508	2.005101
C	10.252695	4.757157	-3.960485
C	11.645417	4.682426	4.175665

C	11.723182	-4.724092	3.970392
C	11.723102	4.724128	-3.970429
C	11.645431	-4.682389	-4.175701
H	10.837336	0.117304	-8.064221
H	10.837416	-0.117277	8.064192
C	10.180063	4.678745	4.156976
C	10.180077	-4.678724	-4.156999
Ag	8.073154	4.569342	4.273210
Ag	8.073167	-4.569337	-4.273214
C	6.064105	4.563988	4.350324
C	6.064117	-4.563996	-4.350310
C	4.822561	4.572724	4.346506
C	4.822573	-4.572739	-4.346482
Ag	2.815216	4.600814	4.248700
Ag	2.815228	-4.600835	-4.248666

**C3**

E= -7096.3394644

v= 1.3415

B	-5.571616	0.101714	5.952141
B	-5.351731	-5.731620	1.653642
C	-5.546758	2.676227	6.118260
H	-5.538541	3.193405	7.079069
C	-5.385151	-6.646336	-0.758212
H	-5.394274	-7.716358	-0.971847
B	-5.457025	-4.089382	5.532559
C	-5.413385	-4.694032	4.151388
C	-5.383656	-5.183086	3.027738
C	-5.502807	-2.591004	5.699861
C	-5.535324	-1.372944	5.833687
C	-5.416077	-5.799891	-1.921964
C	-5.449348	-5.088266	-2.907710
C	-5.486635	-4.278010	-4.001079
C	-5.518927	-3.541950	-4.968740
C	-4.727849	-6.212205	0.462657
C	-4.733336	1.366861	6.079331
B	-5.571609	-0.101747	-5.952139
B	-5.351669	5.731584	-1.653639
C	-5.546779	-2.676261	-6.118256
H	-5.538568	-3.193439	-7.079064
C	-5.385083	6.646299	0.758215
H	-5.394193	7.716322	0.971851
B	-5.456973	4.089348	-5.532556
C	-5.413329	4.693997	-4.151385
C	-5.383596	5.183051	-3.027735
C	-5.502771	2.590970	-5.699859
C	-5.535301	1.372911	-5.833685
C	-5.416022	5.799854	1.921968
C	-5.449302	5.088231	2.907714
C	-5.486598	4.277976	4.001084
C	-5.518897	3.541917	4.968745
C	-4.727783	6.212160	-0.462652
C	-4.733343	-1.366903	-6.079329
B	-16.443192	0.226913	5.926806
B	-16.481715	-5.723674	1.768843
C	-16.502565	2.771144	6.036759
H	-16.522655	3.312962	6.985229
C	-16.490259	-6.684969	-0.626322
H	-16.462610	-7.758302	-0.820720
B	-16.359722	-3.979107	5.604387
C	-16.399640	-4.622399	4.237912
C	-16.434849	-5.142341	3.128325
C	-16.385781	-2.480453	5.737200
C	-16.410718	-1.259327	5.841928
C	-16.507106	-5.857449	-1.803538
C	-16.510757	-5.157836	-2.798736
C	-16.512150	-4.359778	-3.902416
C	-16.510684	-3.634210	-4.878290

C	-17.125697	-6.243972	0.604272
C	-17.209520	1.466802	5.994339
B	-16.443203	-0.226834	-5.926778
B	-16.481659	5.723754	-1.768816
C	-16.502597	-2.771065	-6.036732
H	-16.522690	-3.312883	-6.985202
C	-16.490183	6.685049	0.626349
H	-16.462518	7.758381	0.820747
B	-16.359696	3.979185	-5.604360
C	-16.399605	4.622477	-4.237885
C	-16.434804	5.142420	-3.128298
C	-16.385769	2.480531	-5.737172
C	-16.410716	1.259405	-5.841901
C	-16.507037	5.857528	1.803566
C	-16.510695	5.157915	2.798763
C	-16.512099	4.359856	3.902442
C	-16.510642	3.634288	4.878317
C	-17.125630	6.244060	-0.604243
C	-17.209541	-1.466718	-5.994313
C	-6.193428	-6.226016	0.484801
C	-6.198788	-1.379623	-6.061204
C	-6.193362	6.225989	-0.484799
C	-6.198781	1.379597	6.061208
C	-15.739164	1.500725	6.008235
C	-15.660459	-6.227713	0.590207
C	-15.660393	6.227781	-0.590182
C	-15.739186	-1.500653	-6.008206
C	-10.302084	-6.245618	0.792158
C	-10.302018	6.245641	-0.792152
C	-11.543532	6.241350	-0.803929
C	-11.543598	-6.241323	0.803939
H	-5.455017	4.795712	-6.492113
H	-16.316983	4.668048	-6.576627
H	-16.317014	-4.667971	6.576654
H	-5.455079	-4.795746	6.492116
Ag	-8.295173	6.214862	-0.690671
Ag	-13.553001	6.203907	-0.743792
Ag	-13.553066	-6.203863	0.743810
Ag	-8.295239	-6.214861	0.690673
B	16.443063	0.226866	5.926859
B	16.481684	-5.723688	1.768849
C	16.502424	2.771097	6.036836
H	16.522487	3.312907	6.985311
C	16.490268	-6.684962	-0.626324
H	16.462619	-7.758293	-0.820732
B	16.359617	-3.979152	5.604404
C	16.399563	-4.622432	4.237925
C	16.434793	-5.142366	3.128335
C	16.385667	-2.480498	5.737230
C	16.410597	-1.259373	5.841968
C	16.507139	-5.857431	-1.803533
C	16.510812	-5.157808	-2.798723
C	16.512235	-4.359736	-3.902393
C	16.510795	-3.634156	-4.878260
C	17.125685	-6.243977	0.604285
C	17.209385	1.466758	5.994423
B	16.443338	-0.226773	-5.926722
B	16.481693	5.723780	-1.768711
C	16.502740	-2.771002	-6.036695
H	16.522860	-3.312812	-6.985169
C	16.490165	6.685053	0.626463
H	16.462496	7.758384	0.820870
B	16.359817	3.979244	-5.604273
C	16.399693	4.622525	-4.237792
C	16.434868	5.142459	-3.128199
C	16.385894	2.480591	-5.737097
C	16.410846	1.259466	-5.841833
C	16.506995	5.857522	1.803672
C	16.510630	5.157899	2.798863

C	16.512008	4.359829	3.902534
C	16.510527	3.634251	4.878401
C	17.125639	6.244076	-0.604119
C	17.209680	-1.466654	-5.994245
B	5.571613	0.101679	5.952086
B	5.351715	-5.731650	1.653576
C	5.546773	2.676192	6.118209
H	5.538566	3.193368	7.079019
C	5.385142	-6.646365	-0.758278
H	5.394267	-7.716387	-0.971913
B	5.457003	-4.089416	5.532495
C	5.413363	-4.694064	4.151323
C	5.383636	-5.183118	3.027673
C	5.502790	-2.591038	5.699800
C	5.535313	-1.372979	5.833628
C	5.416069	-5.799919	-1.922030
C	5.449340	-5.088293	-2.907775
C	5.486626	-4.278035	-4.001142
C	5.518915	-3.541974	-4.968803
C	4.727836	-6.212235	0.462589
B	5.571612	-0.101769	-5.952192
B	5.351685	5.731558	-1.653684
C	5.546767	-2.676282	-6.118316
H	5.538548	-3.193458	-7.079126
C	5.385084	6.646271	0.758171
H	5.394187	7.716294	0.971807
B	5.456999	4.089325	-5.532602
C	5.413354	4.693974	-4.151431
C	5.383618	5.183026	-3.027781
C	5.502790	2.590948	-5.699907
C	5.535313	1.372889	-5.833735
C	5.416025	5.799825	1.921922
C	5.449308	5.088200	2.907668
C	5.486607	4.277943	4.001036
C	5.518908	3.541883	4.968696
C	4.727791	6.212130	-0.462699
C	15.660448	-6.227713	0.590193
C	15.739325	-1.500592	-6.008180
C	15.660401	6.227796	-0.590090
C	15.739029	1.500675	6.008281
C	6.198787	1.379558	6.061150
C	6.193415	-6.226044	0.484736
C	6.193371	6.225968	-0.484841
C	6.198784	-1.379649	-6.061265
C	11.543585	-6.241331	0.803887
C	11.543544	6.241351	-0.803909
C	10.302030	6.245639	-0.792154
C	10.302071	-6.245638	0.792102
H	16.317125	4.668115	-6.576535
H	5.455049	4.795691	-6.492158
H	5.455053	-4.795782	6.492051
H	16.316890	-4.668023	6.576665
Ag	13.553012	6.203917	-0.743740
Ag	8.295184	6.214852	-0.690695
Ag	8.295226	-6.214887	0.690612
Ag	13.553054	-6.203863	0.743773
C	4.733342	1.366830	6.079285
C	4.733338	-1.366920	-6.079381
Ag	2.629178	1.183206	6.121413
Ag	2.629174	-1.183292	-6.121486
C	0.620800	1.112382	6.172138
C	0.620796	-1.112464	-6.172186
C	-0.620795	1.112383	6.172144
C	-0.620800	-1.112465	-6.172178
Ag	-2.629173	1.183221	6.121441
Ag	-2.629178	-1.183285	-6.121454

**COF-BHC-1**

E=-1332.6362841

B	2.833100	-5.023346	-0.000135
C	2.830009	-2.450785	-0.000055
B	-4.352551	-2.518117	-0.000154
B	-2.938165	-1.700498	-0.000083
B	-4.350318	-4.151879	0.000021
B	-5.768567	-1.703482	-0.000131
C	-0.711417	-0.411971	0.000012
C	-7.998696	-0.420794	-0.000111
C	1.612362	-1.688835	0.000066
C	0.558940	-1.082228	0.000095
C	5.097826	-1.076947	-0.000226
C	4.045773	-1.685915	-0.000137
C	2.831527	-3.750105	-0.724044
C	2.831641	-3.750150	0.723851
C	-1.836029	-1.062873	-0.723952
C	-1.836117	-1.062826	0.723877
C	-4.348726	-5.425032	0.724115
C	-4.348653	-5.425183	-0.723804
C	-6.872430	-1.068935	-0.724042
C	-6.872427	-1.068956	0.723793
C	-4.347336	-6.724433	0.000299
B	8.587448	4.971429	-0.000097
C	7.485427	4.333793	0.723919
C	7.485260	4.333862	-0.723921
B	-11.530153	-6.674244	-0.000101
B	-2.947242	4.957461	-0.000059
C	-1.843465	4.322703	-0.723933
C	-1.843591	4.322569	0.723885
C	-0.660425	1.023529	-0.000062
C	-0.662277	2.239131	-0.000149
C	6.311730	1.031717	-0.000237
C	6.310008	2.247315	0.000032
C	6.360777	3.682796	0.000101
C	-0.717363	3.674478	0.000016
C	5.090339	4.352915	0.000295
C	4.036863	4.959438	0.000443
C	1.603498	4.956822	0.000310
C	0.551476	4.347769	0.000187
Tv	14.365268	0.017165	-0.000113
Tv	7.166702	12.446065	-0.000046

**COF-BHC-2**

E=-2241.199233

B	-19.403912	-11.102114	-0.000992
B	-4.129051	-2.368358	0.000399
B	-7.808023	-8.660821	0.000616
B	-11.414511	-2.338766	-0.004150
C	-7.791115	-11.221774	-0.002976
C	-1.907482	-1.093201	0.000076
C	-13.614445	-1.028383	0.002329
B	-7.781031	-4.455458	-0.001729
C	-9.077330	-3.700224	-0.005715
C	-10.143548	-3.083303	-0.006671
C	-7.792891	-5.955821	0.000957
C	-7.805109	-7.187477	0.002381
C	-6.476983	-3.712833	-0.000269
C	-5.407558	-3.101297	0.000205
C	-12.499942	-1.694975	0.730137
C	-12.503880	-1.694401	-0.730464
C	-3.033199	-1.737379	0.730319
C	-3.031841	-1.740167	-0.729920
C	-7.804348	-9.925968	0.728424
C	-7.802919	-9.923795	-0.731999
B	3.915624	-6.895974	0.013117
C	3.910287	-4.335060	0.015000
C	3.912852	-8.369445	0.009066
C	3.916545	-5.632515	0.744312
C	3.916568	-5.631288	-0.716185
C	-0.636158	-1.754938	0.003053

B	-3.961055	6.874780	-0.015794
C	-1.759451	5.565823	-0.013581
C	-5.231013	7.621210	-0.012715
C	-2.872906	6.231784	0.715415
C	-2.871861	6.231884	-0.745026
B	12.060158	6.902461	0.002349
C	9.836621	5.630599	0.002914
C	13.339351	7.634566	0.001183
C	10.962819	6.274575	0.732739
C	10.962209	6.274856	-0.727306
C	-1.837347	0.338334	-0.002868
C	3.906415	-9.601351	0.003530
C	-6.296217	8.240175	-0.006453
C	14.408284	8.247150	-0.000067
C	-1.728488	4.133024	-0.012174
C	-1.745756	2.907955	-0.009398
C	-1.783460	1.562380	-0.006098
C	-0.479293	6.210338	-0.011963
C	0.596144	6.797287	-0.009405
C	1.764507	7.465981	-0.006317
C	8.566016	6.293433	0.002363
C	7.484667	6.869411	0.001208
C	9.763946	4.199359	0.002614
C	9.712312	2.975301	0.001410
C	9.677403	1.629655	0.000674
C	9.660739	0.404644	0.001756
C	5.116641	-3.561411	0.014424
C	6.167697	-2.931795	0.010772
C	7.335465	-2.262125	0.006835
C	8.409785	-1.673217	0.004716
C	2.692138	-3.580154	0.014040
C	1.627447	-2.974209	0.010635
C	0.447772	-2.325940	0.006642
C	2.815479	8.095643	-0.004694
C	6.306031	7.519552	0.000160
C	5.240200	8.123776	-0.001843
TV	23.304288	0.000000	0.000000
TV	11.809999	20.095783	0.000000

**COF-BHC-3**

E= -3149.6659804

B	-5.286442	8.833749	-0.025579
C	-3.062444	7.558479	-0.024012
C	-6.556299	9.570929	-0.022692
C	-4.189790	8.200693	-0.755449
C	-4.191079	8.199937	0.705266
C	-7.625199	10.190241	-0.017926
C	-8.783921	10.859362	-0.014552
C	-9.856262	11.476860	-0.013314
B	15.045968	8.820346	0.006446
C	12.836070	7.521206	0.007221
C	17.377814	10.187871	0.005340
C	16.311763	9.563885	0.005300
C	9.331775	9.443900	0.001761
C	8.271198	10.080866	-0.000554
C	7.136216	10.788156	-0.001501
C	6.101307	11.450517	-0.001356
C	13.954786	8.178625	-0.723461
C	13.955502	8.178329	0.737502
C	19.599936	11.489749	0.010033
C	18.532414	10.863905	0.007174
C	10.491012	8.776955	0.004768
C	11.563518	8.177251	0.007301
C	3.692038	11.453748	-0.005060
C	2.652294	10.799038	-0.009051
C	1.511813	10.101131	-0.013018
C	0.445417	9.474047	-0.016038
C	-0.719260	8.817364	-0.018876
C	-1.797450	8.228220	-0.021448
B	-26.858149	-15.734983	-0.015750

B	-16.761578	-2.993250	-0.008785
B	-10.812095	-13.165475	-0.000434
B	-5.055263	-2.962620	-0.002492
C	-10.804899	-15.729272	-0.003420
C	-18.991656	-1.728874	-0.012665
C	-2.843588	-1.666500	-0.000748
C	-7.386573	-4.331030	-0.003539
C	-6.321572	-3.705143	-0.003296
C	-10.844968	-10.461751	0.000241
C	-10.825383	-11.697035	0.001493
C	-15.488798	-3.725082	-0.008894
C	-1.572170	-2.324478	0.002153
C	-0.501153	-2.926654	0.004602
C	0.656692	-3.595870	0.008573
C	-3.962058	-2.323794	-0.732065
C	-3.964821	-2.321027	0.728887
C	-17.860410	-2.367166	-0.741636
C	-17.861525	-2.364586	0.719118
C	-10.804397	-14.430606	-0.732018
C	-10.806738	-14.432269	0.728646
B	5.117326	-8.933627	0.023451
C	5.095480	-6.369937	0.026302
C	5.153318	-11.637226	0.018783
C	5.137047	-10.401933	0.020590
C	5.103494	-7.666915	-0.705131
C	5.102385	-7.668581	0.755554
B	-10.899346	-6.389992	-0.006108
C	-10.886401	-7.886508	-0.002722
C	-10.866780	-9.123787	-0.001581
C	-9.607978	-5.633780	-0.004359
C	-8.540326	-5.008301	-0.003858
C	5.179309	-14.212586	0.015689
C	5.168304	-12.975219	0.017282
C	1.716564	-4.234100	0.013765
C	2.852147	-4.940320	0.019606
C	3.888792	-5.599986	0.024569
C	-14.421761	-4.347541	-0.010168
C	-13.266231	-5.022018	-0.010841
C	-12.197191	-5.645093	-0.010922
C	11.792147	-2.375871	0.015580
C	9.546406	-3.616913	0.014652
C	8.478701	-4.241675	0.016483
C	7.337694	-4.938784	0.020604
C	6.298062	-5.593648	0.025305
C	10.712712	-2.962862	0.014743
C	-2.980986	6.129414	-0.023244
C	-2.911707	4.902675	-0.019399
C	-2.850809	3.566741	-0.014664
C	12.788965	6.090451	0.005675
C	12.785655	4.861777	0.004535
C	12.799976	3.524644	0.005105
C	-2.812773	2.330183	-0.010181
C	-2.795931	0.992957	-0.006209
C	-2.795147	-0.235752	-0.003249
C	12.837791	2.288085	0.007673
C	12.899579	0.952396	0.010940
C	12.969920	-0.274264	0.013553
TV	32.047262	0.025873	0.027948
TV	15.702624	27.954577	0.001864

**MOF-BHC-1**

E= -3902.3807209

B	-5.634968	5.886730	0.591171
B	-6.037215	2.093222	-5.547362
C	-5.614534	5.858603	3.174660
H	-5.525053	6.776785	3.778779
C	-6.086034	-0.228307	-6.677716

H	-6.132830	-0.347816	-7.772754	C	-1.304304	1.035343	-6.123719
B	-5.805359	5.791093	-3.592060	C	-1.335580	-1.038393	6.118758
C	-5.881621	4.480768	-4.299153	C	-0.105667	-0.823160	6.131373
C	-5.946674	3.396571	-4.885865	C	-0.074269	0.820548	-6.129991
C	-5.759959	5.839063	-2.106891	H	-5.791595	-6.818114	4.201202
C	-5.714098	5.879436	-0.871870	H	4.188831	-5.555589	5.768089
C	-6.008241	-1.437209	-5.936990	H	4.215378	5.555218	-5.742254
C	-5.913125	-2.485002	-5.306574	H	-5.774207	6.815376	-4.227199
C	-5.802332	-3.625310	-4.602121	Ag	-3.286407	-1.111849	6.124917
C	-5.700612	-4.657810	-3.948155	Ag	1.751028	-0.243069	6.174776
C	-6.698746	0.957725	-6.110348	Ag	1.782925	0.241366	-6.163039
C	-6.403617	5.989693	1.903666	Ag	-3.255090	1.108763	-6.138997
B	-5.629248	-5.889620	-0.616484	C	4.721027	6.251868	0.397989
B	-6.064447	-2.096079	5.519790	C	4.726923	-6.252038	-0.369499
C	-5.596387	-5.861432	-3.199849	Ag	6.710325	6.246018	0.243683
H	-5.503908	-6.779581	-3.803572	Ag	6.715674	-6.245865	-0.208371
C	-6.120622	0.225356	6.649976	C	8.661193	6.232645	0.314732
H	-6.173480	0.344826	7.744741	C	8.666796	-6.232100	-0.272233
B	-5.820162	-5.793885	3.565857	C	9.891227	6.199705	0.527104
C	-5.900813	-4.483556	4.272473	C	9.897641	-6.198776	-0.479764
C	-5.969595	-3.399371	4.858789	Ag	11.747927	6.103207	1.100829
C	-5.767349	-5.841887	2.080942	Ag	11.756636	-6.101776	-1.045847
C	-5.715500	-5.882285	0.846149	TV	19.965676	0.002407	0.045639
C	-6.039449	1.434321	5.909704				
C	-5.941339	2.482139	5.279794				
C	-5.827168	3.622474	4.575921				
C	-5.722324	4.654970	3.922438				
C	-6.729729	-0.960994	6.079231				
C	-6.391494	-5.992603	-1.932709				
B	3.938071	5.848445	-0.850270				
B	4.364265	0.652053	-5.868515				
C	3.870996	6.466952	1.656209				
H	3.813716	7.511959	2.002920				
C	4.388795	-1.876315	-6.400104				
H	4.476504	-2.268773	-7.426861				
B	4.186005	4.716808	-4.876325				
C	4.234931	3.276233	-5.240109				
C	4.282876	2.078811	-5.545033				
C	4.106936	5.130167	-3.446084				
C	4.037121	5.475449	-2.262917				
C	4.284406	-2.865074	-5.384636				
C	4.180286	-3.722873	-4.514294				
C	4.066002	-4.652461	-3.549033				
C	3.967100	-5.489688	-2.658161				
C	5.044100	-0.591058	-6.123085				
B	3.937336	-5.849159	0.874728				
B	4.334297	-0.652371	5.895081				
C	3.883162	-6.467646	-1.632075				
H	3.828385	-7.512692	-1.979068				
C	4.354350	1.875985	6.426911				
H	4.436069	2.268431	7.454167				
B	4.163592	-4.717231	4.901979				
C	4.209846	-3.276621	5.265968				
C	4.255505	-2.079167	5.571120				
C	4.092264	-5.130689	3.471356				
C	4.028815	-5.476049	2.287858				
C	4.254991	2.864730	5.410926				
C	4.155016	3.722474	4.540044				
C	4.045244	4.651961	3.574162				
C	3.950361	5.489068	2.682742				
C	5.011968	0.591123	6.153526				
C	-5.244126	0.959563	-6.195033				
C	-4.945605	-5.865537	-1.882999				
C	-5.275607	-0.961950	6.171817				
C	-4.957484	5.862739	1.860962				
C	3.267323	6.156342	0.374195				
C	3.597687	-0.608557	-6.252508				
C	3.564844	0.607759	6.274815				
C	3.273023	-6.157493	-0.353115				