

Supplementary Materials

Density functional theory study of the regioselectivity in copolymerization of *bis*-styrenic molecules with propylene using zirconocene catalyst

Shu-Yuan Yu,¹ Xiaoxia Peng,¹ Fuping Wang,¹ Jian Cao,¹ Fei Wang,¹ Cheng-Gen Zhang,^{1,2,*}

¹ College of Chemistry and Material Science, Langfang Normal University, Langfang 065000, China

² College of Chemistry and Chemical Engineering, University of Chinese Academy of Sciences, Beijing 100049, China

Correspondence to: C.-G. Zhang (E-mail: chgzhang04@mails.ucas.ac.cn)

Contents

Figure S1: The relative free energy for the insertions of propylene into the Zr–C bond of [Zr]–CH₃.

Figure S2: Optimized structures of the key TSs and intermediates (IMs) shown in Figure S1.

Figure S3: The relative free energy for the insertions of DVB or BVPE into the Zr–C bond of [Zr]–PP₁.

Figure S4: Optimized structures of the key TSs and products shown in Figure S3.

Figure S5: The relative free energy for the insertions of propylene into the Zr–C bond of [Zr]–DVB–PP₁ or [Zr]–BVPE–PP₁.

Figure S6: Optimized structures of the key TSs and intermediates (IMs) shown in Figure S5.

Table S1: Detailed data of the local reactivity index and fukui functions values for some molecules.

Table S2: Energies and cartesian coordinates of all the structures.

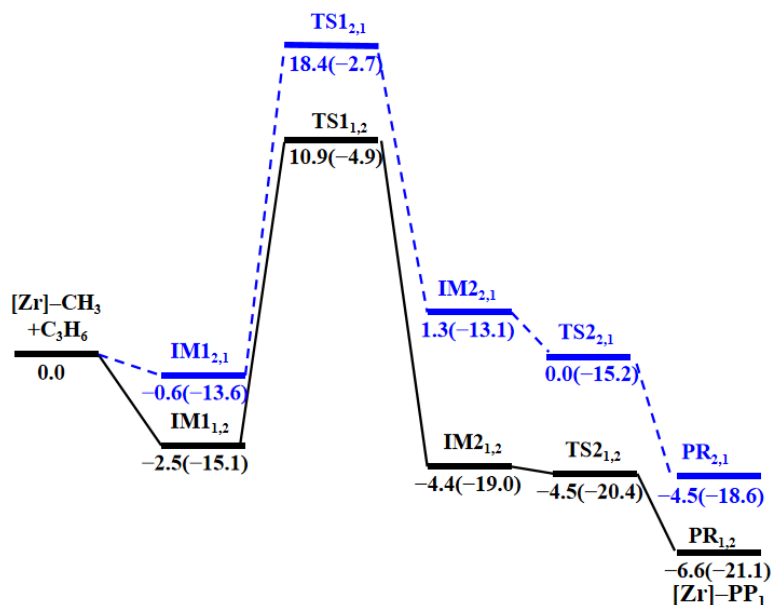


Figure S1. The relative free energy for the insertions of propylene into the Zr-C bond of [Zr]-CH₃ (in kcal/mol), and the relative enthalpy is also given in parentheses for reference (in kcal/mol). The black and blue pathways represent the 1,2- and 2,1-insertion, respectively.

The pathways for the insertions of propylene into the Zr-C bond of [Zr]-CH₃.

Briefly, propylene prefers 1,2-insertion over 2,1-insertion both kinetically and thermodynamically, explaining the observed 1,2-insertion regioselectivity for propylene insertion. Relative to the complex before the transition state, the barrier for 1,2-insertion is 13.4 kcal/mol, compared with the 19.0 kcal/mol for 2,1-insertion. The 1,2-insertion is over all exergonic by 6.6 kcal/mol, compared with the exergonic 4.5 kcal/mol for 2,1-insertion. The kinetic and thermodynamic preference of 1,2- over 2,1-insertion is in agreement with the observed 1,2-insertion regioselectivity in the propylene polymerization.

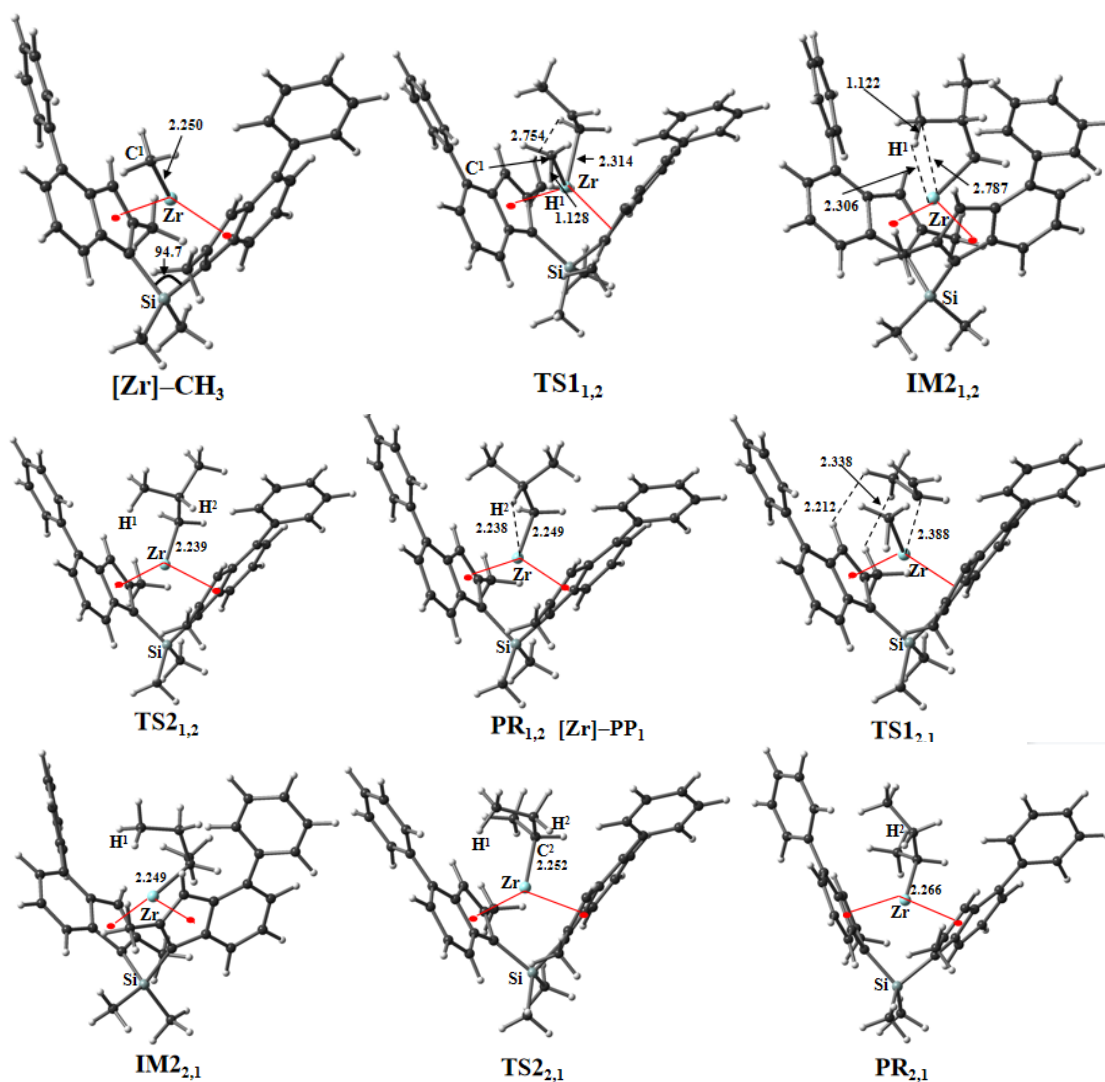


Figure S2. Optimized structures of the key TSs and intermediates (IMs) shown in Figure S1. Key bond lengths are given in angstrom.

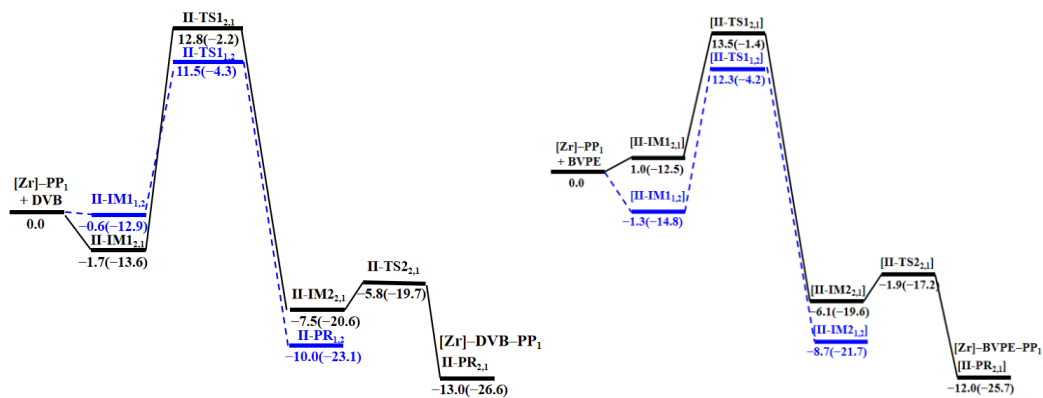
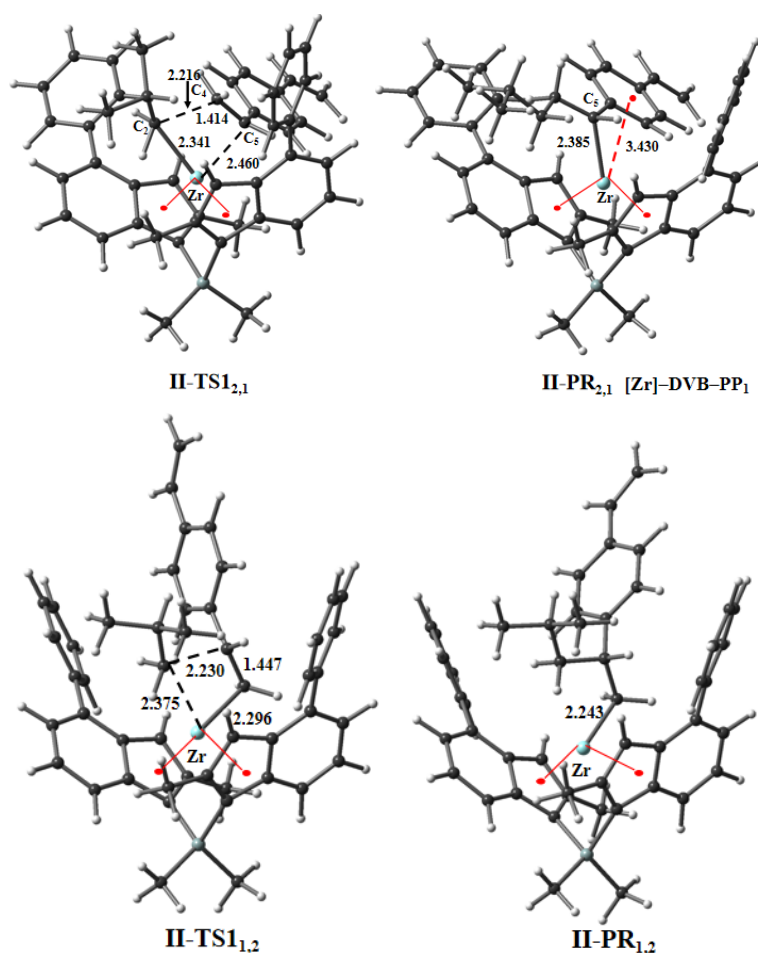


Figure S3. The relative free energy for the insertions of DVB or BVPE into the Zr-C bond of [Zr]-PP₁ (in kcal/mol), and the relative enthalpy is also given in parentheses

for reference (in kcal/mol). The black and blue pathways represent the 1,2- and 2,1-insertion, respectively.

The pathways for the insertions of DVB or BVPE into the Zr–C bond of [Zr]–PP₁. The 2,1-insertion of DVB [BVPE] is kinetically slightly less favorable but thermodynamically more favorable than 1,2-insertion. The observation of 2,1-insertion DVB [BVPE] at the end of polymer chain is due to thermodynamic control.

Overall, the 2,1-insertion is thermodynamically more favorable than 1,2-insertion by 3.0 [3.3] kcal/mol, Although the 1,2-insertion is kinetically slightly more favorable than the 2,1-insertion, the reaction would result in due to [Zr]–DVB–PP₁ [or [Zr]–BVPE–PP₁] thermodynamic control.



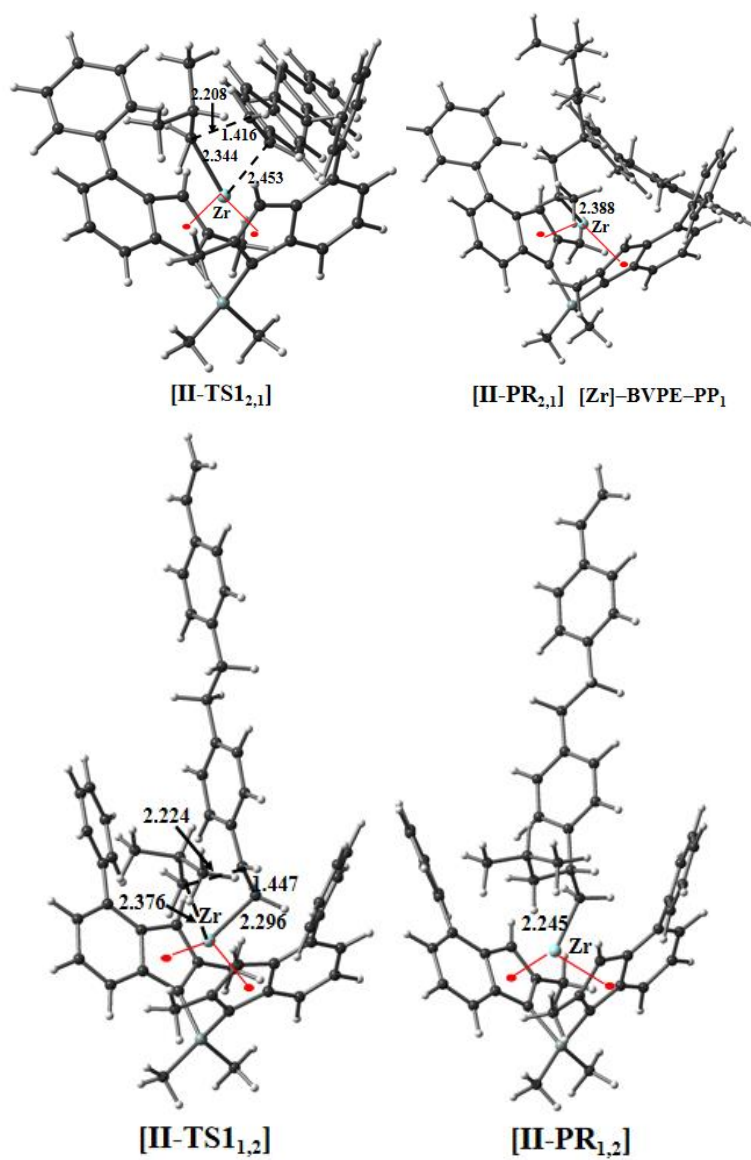


Figure S4. Optimized structures of the key TSs and products shown in Figure S3. Key bond lengths are given in angstrom.

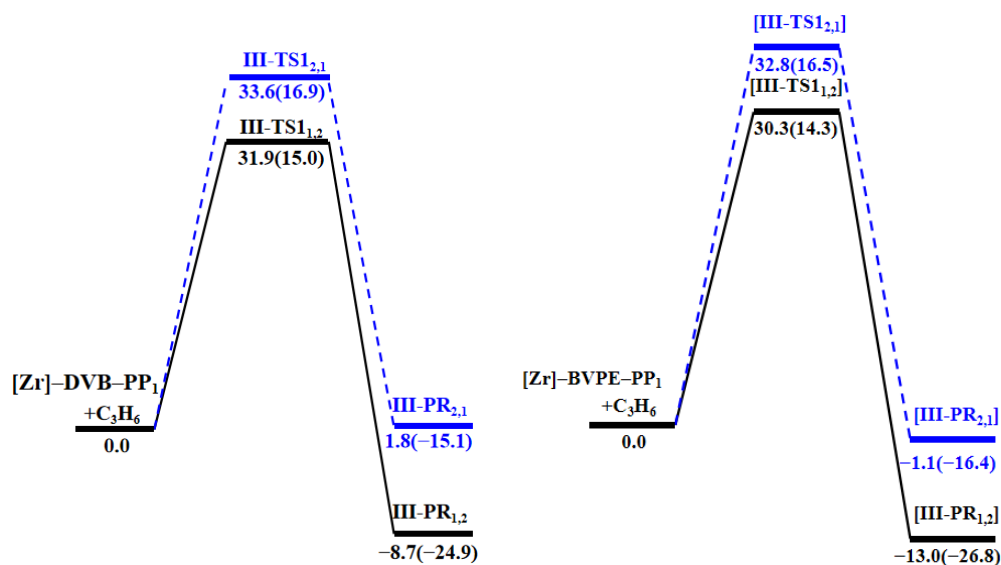
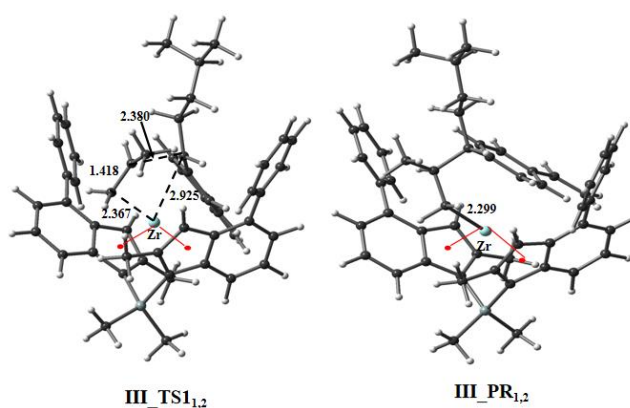


Figure S5. The relative free energy for the insertions of propylene into the Zr–C bond of [Zr]–DVB–PP₁ or [Zr]–BVPE–PP₁ (in kcal/mol), and the relative enthalpy is also given in parentheses for reference (in kcal/mol). The black and blue pathways represent the 1,2- and 2,1-insertion, respectively.

The pathways for the insertions of propylene into the Zr–C bond of [Zr]–DVB–PP₁ or [Zr]–BVPE–PP₁. Briefly, the barriers for propylene 1,2- and 2,1-insertions for [Zr]–DVB–PP₁ and [Zr]–BVPE–PP₁ are 31.9 [33.6] and 30.3 [32.8] kcal/mol, respectively, which are much higher than those for propylene insertions into [Zr]–PP₁. The high barriers indicates the insertion of a DVB[BVPE] explain would hinder subsequent insertion of either propylene, deactivating the catalytic system.



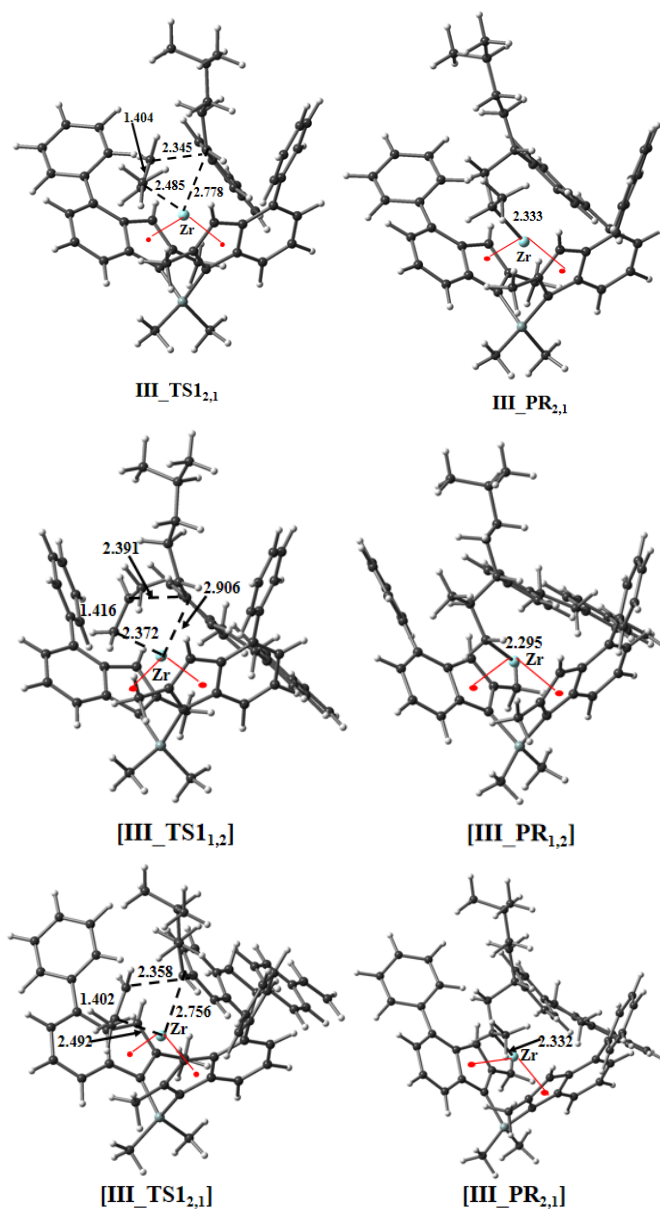


Figure S6. Optimized structures of the key TSs and products shown in Figure S5. Key bond lengths are given in angstrom.

Table S1: Detailed data of the local reactivity index values and fukui functions values for some molecules.

[Zr]-DVB-PP₁

Condensed local electrophilicity/nucleophilicity index (e*eV)

Atom	Electrophilicity	Nucleophilicity
1(C)	0.07793	0.02576
2(C)	0.15259	0.04021
3(C)	0.02212	0.01196
4(C)	0.02528	0.00432
5(C)	0.07637	0.02124

6(C)	0.02417	0.00135
7(Zr)	0.84212	0.00875
8(C)	0.05956	0.01440
9(C)	0.03422	0.00507
10(C)	0.05893	0.00583
11(C)	0.03179	0.00476
12(C)	0.07190	0.01569
13(Si)	0.03069	0.00573
14(C)	0.02433	0.00541
15(C)	0.03262	0.00586
16(C)	0.10364	0.01252
17(C)	0.02412	0.01617
18(C)	0.08156	0.01962
19(C)	0.15595	0.01683
20(C)	0.04049	0.00511
21(C)	0.03274	0.00402
22(C)	-0.03549	-0.00210
23(C)	0.05114	0.02729
24(C)	0.01421	0.04236
25(C)	0.07384	0.03729
26(C)	0.11320	0.02442
27(C)	-0.02714	0.00889
28(C)	0.01714	0.00521
29(C)	0.05738	0.01163
30(C)	0.09074	0.01947
31(C)	0.01290	0.00298
32(C)	0.05322	0.01062
33(C)	-0.01717	0.01000
34(C)	0.03025	0.01682
35(C)	0.08325	0.03640
36(C)	0.03613	0.01820
37(C)	0.06822	0.02134
38(C)	0.01599	0.00403
39(C)	0.00138	0.00059
40(C)	0.00945	0.00140
41(C)	0.04714	0.00486
42(C)	0.01657	0.00960
43(C)	0.02641	0.01693
44(C)	0.11057	0.02207
45(C)	0.08633	0.01714
46(C)	0.11415	0.01115
47(C)	0.01660	0.00356
48(H)	0.04341	0.00813
49(H)	0.05266	0.00797
50(H)	0.05049	0.00847
51(H)	0.00454	0.00199
52(H)	0.04823	0.00944
53(H)	0.04857	0.00814
54(H)	0.04900	0.01057
55(H)	0.02012	0.00221
56(H)	0.03999	0.00828
57(H)	0.07062	0.01228
58(H)	0.08828	0.01214
59(H)	0.03202	0.01510
60(H)	0.05977	0.01696
61(H)	0.07530	0.01784
62(H)	0.01222	0.00342

63(H)	0.04957	0.00960
64(H)	0.06063	0.01173
65(H)	0.00499	0.00111
66(H)	0.04625	0.00873
67(H)	-0.02323	0.00135
68(H)	0.02450	0.01153
69(H)	0.05688	0.01849
70(H)	0.02690	0.01049
71(H)	0.05436	0.01604
72(H)	0.03376	0.00387
73(H)	0.02467	0.00454
74(H)	0.09229	0.01147
75(H)	0.02698	0.00255
76(H)	0.03520	0.00380
77(H)	0.07554	0.01195
78(H)	0.01646	-0.00034
79(H)	-0.01295	-0.00278
80(H)	0.00815	0.00364
81(H)	0.01200	0.00635
82(H)	0.03223	0.00902
83(H)	0.05659	0.00876
84(H)	0.07638	0.01074
85(H)	0.03477	0.00908
86(H)	0.06414	0.01340
87(C)	0.01031	0.00137
88(H)	0.04576	0.00876
89(H)	0.00671	0.00118
90(H)	0.01337	0.00384
91(H)	0.02682	0.00543
92(H)	0.04812	0.00970
93(H)	-0.00291	-0.00256
94(H)	-0.00147	-0.00216
95(C)	0.06438	0.00983
96(H)	0.05012	0.01112
97(C)	0.06692	0.02752
98(H)	0.03309	0.01015
99(H)	0.08511	0.01856

Hirshfeld charges, condensed Fukui functions Units used below are "e" (elementary charge)

Atom	q(N)	q(N+1)	q(N-1)	f-	f+	f0
1(C)	-0.1296	-0.1449	-0.1054	0.0242	0.0153	0.0198
2(C)	-0.0662	-0.0962	-0.0284	0.0378	0.0300	0.0339
3(C)	-0.0376	-0.0420	-0.0264	0.0112	0.0043	0.0078
4(C)	-0.0226	-0.0275	-0.0185	0.0041	0.0050	0.0045
5(C)	-0.0555	-0.0705	-0.0355	0.0200	0.0150	0.0175
6(C)	-0.0021	-0.0069	-0.0008	0.0013	0.0047	0.0030
7(Zr)	0.5069	0.3414	0.5152	0.0082	0.1655	0.0869
8(C)	-0.1378	-0.1495	-0.1242	0.0135	0.0117	0.0126
9(C)	-0.0269	-0.0337	-0.0222	0.0048	0.0067	0.0057
10(C)	0.0046	-0.0070	0.0101	0.0055	0.0116	0.0085
11(C)	-0.0129	-0.0192	-0.0084	0.0045	0.0062	0.0054
12(C)	-0.0569	-0.0711	-0.0422	0.0148	0.0141	0.0144
13(Si)	0.3745	0.3684	0.3798	0.0054	0.0060	0.0057

14(C)	-0.1712	-0.1759	-0.1661	0.0051	0.0048	0.0049
15(C)	-0.1693	-0.1757	-0.1638	0.0055	0.0064	0.0060
16(C)	0.0230	0.0026	0.0347	0.0118	0.0204	0.0161
17(C)	-0.0273	-0.0320	-0.0121	0.0152	0.0047	0.0100
18(C)	-0.0262	-0.0422	-0.0077	0.0184	0.0160	0.0172
19(C)	-0.0233	-0.0539	-0.0074	0.0158	0.0306	0.0232
20(C)	-0.0686	-0.0766	-0.0638	0.0048	0.0080	0.0064
21(C)	-0.0702	-0.0766	-0.0664	0.0038	0.0064	0.0051
22(C)	-0.0031	0.0038	-0.0051	-0.0020	-0.0070	-0.0045
23(C)	0.0172	0.0071	0.0429	0.0257	0.0101	0.0179
24(C)	-0.0301	-0.0329	0.0098	0.0398	0.0028	0.0213
25(C)	-0.0266	-0.0411	0.0085	0.0351	0.0145	0.0248
26(C)	-0.0273	-0.0495	-0.0043	0.0230	0.0222	0.0226
27(C)	-0.0027	0.0027	0.0057	0.0084	-0.0053	0.0015
28(C)	-0.0368	-0.0402	-0.0319	0.0049	0.0034	0.0041
29(C)	-0.0310	-0.0422	-0.0200	0.0109	0.0113	0.0111
30(C)	-0.0250	-0.0428	-0.0067	0.0183	0.0178	0.0181
31(C)	-0.0374	-0.0400	-0.0346	0.0028	0.0025	0.0027
32(C)	-0.0303	-0.0408	-0.0204	0.0100	0.0105	0.0102
33(C)	-0.0475	-0.0441	-0.0381	0.0094	-0.0034	0.0030
34(C)	-0.0380	-0.0440	-0.0222	0.0158	0.0059	0.0109
35(C)	-0.0279	-0.0443	0.0063	0.0342	0.0164	0.0253
36(C)	-0.0343	-0.0414	-0.0172	0.0171	0.0071	0.0121
37(C)	-0.0303	-0.0437	-0.0102	0.0201	0.0134	0.0167
38(C)	-0.0473	-0.0504	-0.0435	0.0038	0.0031	0.0035
39(C)	-0.0460	-0.0463	-0.0455	0.0006	0.0003	0.0004
40(C)	-0.0107	-0.0126	-0.0094	0.0013	0.0019	0.0016
41(C)	0.0097	0.0004	0.0143	0.0046	0.0093	0.0069
42(C)	-0.0748	-0.0781	-0.0658	0.0090	0.0033	0.0061
43(C)	-0.0106	-0.0157	0.0054	0.0159	0.0052	0.0106
44(C)	0.0059	-0.0158	0.0266	0.0208	0.0217	0.0212
45(C)	-0.0212	-0.0382	-0.0051	0.0161	0.0170	0.0165
46(C)	-0.0089	-0.0314	0.0015	0.0105	0.0224	0.0165
47(C)	-0.0853	-0.0885	-0.0819	0.0033	0.0033	0.0033
48(H)	0.0526	0.0441	0.0603	0.0076	0.0085	0.0081
49(H)	0.0578	0.0475	0.0653	0.0075	0.0103	0.0089
50(H)	0.0476	0.0377	0.0556	0.0080	0.0099	0.0089
51(H)	0.0350	0.0341	0.0369	0.0019	0.0009	0.0014
52(H)	0.0473	0.0378	0.0562	0.0089	0.0095	0.0092
53(H)	0.0485	0.0390	0.0561	0.0077	0.0095	0.0086
54(H)	0.0479	0.0383	0.0579	0.0099	0.0096	0.0098
55(H)	0.0383	0.0344	0.0404	0.0021	0.0040	0.0030
56(H)	0.0515	0.0437	0.0593	0.0078	0.0079	0.0078
57(H)	0.0551	0.0412	0.0667	0.0115	0.0139	0.0127

58(H)	0.0575	0.0402	0.0690	0.0114	0.0173	0.0144
59(H)	0.0471	0.0408	0.0613	0.0142	0.0063	0.0102
60(H)	0.0507	0.0390	0.0667	0.0159	0.0117	0.0138
61(H)	0.0558	0.0410	0.0726	0.0168	0.0148	0.0158
62(H)	0.0447	0.0423	0.0479	0.0032	0.0024	0.0028
63(H)	0.0537	0.0440	0.0628	0.0090	0.0097	0.0094
64(H)	0.0559	0.0440	0.0669	0.0110	0.0119	0.0115
65(H)	0.0430	0.0421	0.0441	0.0010	0.0010	0.0010
66(H)	0.0541	0.0450	0.0623	0.0082	0.0091	0.0087
67(H)	0.0268	0.0314	0.0281	0.0013	-0.0046	-0.0016
68(H)	0.0462	0.0413	0.0570	0.0108	0.0048	0.0078
69(H)	0.0542	0.0430	0.0716	0.0174	0.0112	0.0143
70(H)	0.0450	0.0397	0.0548	0.0099	0.0053	0.0076
71(H)	0.0539	0.0432	0.0690	0.0151	0.0107	0.0129
72(H)	0.0459	0.0392	0.0495	0.0036	0.0066	0.0051
73(H)	0.0361	0.0312	0.0403	0.0043	0.0048	0.0046
74(H)	0.0535	0.0354	0.0643	0.0108	0.0181	0.0145
75(H)	0.0443	0.0390	0.0467	0.0024	0.0053	0.0039
76(H)	0.0395	0.0326	0.0431	0.0036	0.0069	0.0052
77(H)	0.0524	0.0376	0.0637	0.0112	0.0148	0.0130
78(H)	0.0261	0.0229	0.0258	-0.0003	0.0032	0.0015
79(H)	0.0208	0.0233	0.0182	-0.0026	-0.0025	-0.0026
80(H)	0.0257	0.0241	0.0291	0.0034	0.0016	0.0025
81(H)	0.0340	0.0317	0.0400	0.0060	0.0024	0.0042
82(H)	0.0505	0.0442	0.0590	0.0085	0.0063	0.0074
83(H)	0.0551	0.0440	0.0633	0.0082	0.0111	0.0097
84(H)	0.0560	0.0410	0.0661	0.0101	0.0150	0.0126
85(H)	0.0307	0.0238	0.0392	0.0085	0.0068	0.0077
86(H)	0.0316	0.0189	0.0442	0.0126	0.0126	0.0126
87(C)	-0.0862	-0.0882	-0.0849	0.0013	0.0020	0.0017
88(H)	0.0353	0.0263	0.0435	0.0082	0.0090	0.0086
89(H)	0.0264	0.0251	0.0275	0.0011	0.0013	0.0012
90(H)	0.0291	0.0265	0.0327	0.0036	0.0026	0.0031
91(H)	0.0287	0.0235	0.0339	0.0051	0.0053	0.0052
92(H)	0.0351	0.0256	0.0442	0.0091	0.0095	0.0093
93(H)	0.0291	0.0296	0.0267	-0.0024	-0.0006	-0.0015
94(H)	0.0241	0.0244	0.0221	-0.0020	-0.0003	-0.0012
95(C)	-0.0082	-0.0209	0.0010	0.0092	0.0127	0.0109
96(H)	0.0495	0.0397	0.0600	0.0105	0.0098	0.0102
97(C)	-0.1386	-0.1518	-0.1128	0.0259	0.0132	0.0195
98(H)	0.0428	0.0363	0.0524	0.0095	0.0065	0.0080
99(H)	0.0559	0.0392	0.0734	0.0174	0.0167	0.0171

[Zr]-[BVPE]-PP₁

Condensed local electrophilicity/nucleophilicity index (e*eV)

Atom	Electrophilicity	Nucleophilicity
1(C)	0.08364	0.01317
2(C)	0.05649	0.12207
3(C)	0.00399	0.06367
4(C)	0.02521	0.00480
5(C)	0.07830	0.02162
6(C)	0.02476	0.00125
7(Zr)	0.85441	0.00627
8(C)	0.06048	0.01533
9(C)	0.03412	0.00540
10(C)	0.05953	0.00712
11(C)	0.03071	0.00504
12(C)	0.07296	0.02014
13(Si)	0.03171	0.00598
14(C)	0.02499	0.00509
15(C)	0.03242	0.00638
16(C)	0.10438	0.01442
17(C)	0.02595	0.01569
18(C)	0.08262	0.01764
19(C)	0.16067	0.01453
20(C)	0.04186	0.00368
21(C)	0.03295	0.00458
22(C)	-0.03598	-0.00171
23(C)	0.05488	0.02832
24(C)	0.01394	0.04373
25(C)	0.07382	0.03651
26(C)	0.11619	0.02728
27(C)	-0.02753	0.01043
28(C)	0.01678	0.00665
29(C)	0.05749	0.01348
30(C)	0.09109	0.02146
31(C)	0.01309	0.00245
32(C)	0.05364	0.01063
33(C)	-0.01543	0.00941
34(C)	0.03195	0.01504
35(C)	0.08435	0.03659
36(C)	0.03638	0.02049
37(C)	0.06840	0.02248
38(C)	0.01677	0.00223
39(C)	0.00094	0.00044
40(C)	0.00939	0.00132
41(C)	0.05231	0.00540

42(C)	0.02190	0.00593
43(C)	0.04445	0.00573
44(C)	0.11615	0.00530
45(C)	0.07424	0.01144
46(C)	0.12408	0.00683
47(C)	0.01686	0.00370
48(H)	0.04615	0.00641
49(H)	0.05302	0.00961
50(H)	0.05062	0.00827
51(H)	0.00598	0.00036
52(H)	0.04863	0.01014
53(H)	0.04971	0.00871
54(H)	0.04839	0.01124
55(H)	0.01944	0.00278
56(H)	0.04147	0.00744
57(H)	0.07173	0.01106
58(H)	0.09142	0.00936
59(H)	0.03200	0.01590
60(H)	0.06015	0.01759
61(H)	0.07610	0.01950
62(H)	0.01214	0.00424
63(H)	0.04961	0.01119
64(H)	0.06073	0.01310
65(H)	0.00569	-0.00048
66(H)	0.04657	0.00846
67(H)	-0.02211	0.00117
68(H)	0.02605	0.00919
69(H)	0.05735	0.01844
70(H)	0.02680	0.01199
71(H)	0.05448	0.01739
72(H)	0.04086	-0.00031
73(H)	0.02636	0.00363
74(H)	0.09249	0.00999
75(H)	0.02672	0.00324
76(H)	0.03571	0.00437
77(H)	0.07587	0.01302
78(H)	0.01725	-0.00185
79(H)	-0.01316	-0.00326
80(H)	0.00885	0.00337
81(H)	0.01322	0.00471
82(H)	0.03712	0.00346
83(H)	0.05276	0.00809
84(H)	0.07817	0.00692
85(H)	0.03748	0.00692

86(H)	0.06561	0.01004
87(C)	0.01026	0.00127
88(H)	0.04592	0.00930
89(H)	0.00699	0.00128
90(H)	0.01381	0.00396
91(H)	0.02695	0.00534
92(H)	0.04852	0.01013
93(H)	-0.00321	-0.00340
94(H)	-0.00158	-0.00234
95(C)	0.01480	0.00750
96(H)	0.03721	0.00496
97(C)	0.00061	0.00921
98(H)	-0.01449	0.01168
99(H)	0.04945	0.00745
100(H)	0.00266	0.01435
101(C)	-0.03863	0.06163
102(C)	-0.01272	0.03095
103(C)	0.00147	0.03684
104(C)	0.01633	0.04302
105(H)	-0.01492	0.02206
106(C)	0.02356	0.04681
107(H)	0.00061	0.02533
108(C)	0.03538	0.04792
109(H)	0.01650	0.02203
110(H)	0.02487	0.02756
111(C)	0.06665	0.00811
112(H)	0.01694	0.03098
113(C)	0.06728	0.02543
114(H)	0.03316	0.04429
115(H)	0.01349	0.03431

Hirshfeld charges, condensed Fukui functions, Units used below are "e" (elementary charge)

Atom	q(N)	q(N+1)	q(N-1)	f-	f+	f0
1(C)	-0.1313	-0.1476	-0.1232	0.0081	0.0163	0.0122
2(C)	-0.0777	-0.0887	-0.0023	0.0754	0.0110	0.0432
3(C)	-0.0392	-0.0400	0.0001	0.0393	0.0008	0.0201
4(C)	-0.0232	-0.0281	-0.0202	0.0030	0.0049	0.0039
5(C)	-0.0559	-0.0712	-0.0425	0.0134	0.0153	0.0143
6(C)	-0.0023	-0.0071	-0.0015	0.0008	0.0048	0.0028
7(Zr)	0.5074	0.3408	0.5113	0.0039	0.1666	0.0852
8(C)	-0.1382	-0.1499	-0.1287	0.0095	0.0118	0.0106
9(C)	-0.0274	-0.0340	-0.0240	0.0033	0.0067	0.0050
10(C)	0.0045	-0.0071	0.0089	0.0044	0.0116	0.0080
11(C)	-0.0132	-0.0192	-0.0101	0.0031	0.0060	0.0046

12(C)	-0.0568	-0.0710	-0.0444	0.0124	0.0142	0.0133
13(Si)	0.3745	0.3683	0.3782	0.0037	0.0062	0.0049
14(C)	-0.1714	-0.1762	-0.1682	0.0031	0.0049	0.0040
15(C)	-0.1695	-0.1758	-0.1655	0.0039	0.0063	0.0051
16(C)	0.0228	0.0024	0.0317	0.0089	0.0204	0.0146
17(C)	-0.0271	-0.0322	-0.0174	0.0097	0.0051	0.0074
18(C)	-0.0267	-0.0428	-0.0158	0.0109	0.0161	0.0135
19(C)	-0.0234	-0.0547	-0.0144	0.0090	0.0313	0.0202
20(C)	-0.0686	-0.0767	-0.0663	0.0023	0.0082	0.0052
21(C)	-0.0704	-0.0768	-0.0675	0.0028	0.0064	0.0046
22(C)	-0.0030	0.0040	-0.0041	-0.0011	-0.0070	-0.0040
23(C)	0.0173	0.0066	0.0348	0.0175	0.0107	0.0141
24(C)	-0.0301	-0.0328	-0.0031	0.0270	0.0027	0.0149
25(C)	-0.0266	-0.0410	-0.0040	0.0226	0.0144	0.0185
26(C)	-0.0272	-0.0498	-0.0103	0.0169	0.0227	0.0198
27(C)	-0.0028	0.0026	0.0036	0.0064	-0.0054	0.0005
28(C)	-0.0368	-0.0401	-0.0327	0.0041	0.0033	0.0037
29(C)	-0.0312	-0.0424	-0.0228	0.0083	0.0112	0.0098
30(C)	-0.0254	-0.0432	-0.0121	0.0133	0.0178	0.0155
31(C)	-0.0377	-0.0402	-0.0362	0.0015	0.0026	0.0020
32(C)	-0.0307	-0.0411	-0.0241	0.0066	0.0105	0.0085
33(C)	-0.0476	-0.0446	-0.0418	0.0058	-0.0030	0.0014
34(C)	-0.0382	-0.0444	-0.0289	0.0093	0.0062	0.0078
35(C)	-0.0282	-0.0447	-0.0056	0.0226	0.0164	0.0195
36(C)	-0.0345	-0.0416	-0.0218	0.0127	0.0071	0.0099
37(C)	-0.0306	-0.0439	-0.0167	0.0139	0.0133	0.0136
38(C)	-0.0473	-0.0506	-0.0460	0.0014	0.0033	0.0023
39(C)	-0.0462	-0.0464	-0.0459	0.0003	0.0002	0.0002
40(C)	-0.0107	-0.0125	-0.0099	0.0008	0.0018	0.0013
41(C)	0.0091	-0.0011	0.0124	0.0033	0.0102	0.0068
42(C)	-0.0766	-0.0809	-0.0729	0.0037	0.0043	0.0040
43(C)	-0.0213	-0.0299	-0.0177	0.0035	0.0087	0.0061
44(C)	0.0112	-0.0115	0.0144	0.0033	0.0226	0.0130
45(C)	-0.0212	-0.0357	-0.0141	0.0071	0.0145	0.0108
46(C)	-0.0105	-0.0347	-0.0063	0.0042	0.0242	0.0142
47(C)	-0.0852	-0.0885	-0.0830	0.0023	0.0033	0.0028
48(H)	0.0521	0.0431	0.0561	0.0040	0.0090	0.0065
49(H)	0.0576	0.0473	0.0636	0.0059	0.0103	0.0081
50(H)	0.0472	0.0374	0.0523	0.0051	0.0099	0.0075
51(H)	0.0350	0.0338	0.0352	0.0002	0.0012	0.0007
52(H)	0.0474	0.0380	0.0537	0.0063	0.0095	0.0079
53(H)	0.0484	0.0387	0.0537	0.0054	0.0097	0.0075
54(H)	0.0476	0.0382	0.0546	0.0069	0.0094	0.0082
55(H)	0.0383	0.0345	0.0400	0.0017	0.0038	0.0028

56(H)	0.0515	0.0434	0.0561	0.0046	0.0081	0.0063
57(H)	0.0546	0.0406	0.0615	0.0068	0.0140	0.0104
58(H)	0.0576	0.0398	0.0634	0.0058	0.0178	0.0118
59(H)	0.0470	0.0408	0.0569	0.0098	0.0062	0.0080
60(H)	0.0507	0.0390	0.0616	0.0109	0.0117	0.0113
61(H)	0.0556	0.0407	0.0676	0.0120	0.0148	0.0134
62(H)	0.0447	0.0423	0.0473	0.0026	0.0024	0.0025
63(H)	0.0536	0.0439	0.0605	0.0069	0.0097	0.0083
64(H)	0.0556	0.0438	0.0637	0.0081	0.0118	0.0100
65(H)	0.0427	0.0416	0.0424	-0.0003	0.0011	0.0004
66(H)	0.0537	0.0446	0.0589	0.0052	0.0091	0.0072
67(H)	0.0268	0.0312	0.0276	0.0007	-0.0043	-0.0018
68(H)	0.0463	0.0412	0.0520	0.0057	0.0051	0.0054
69(H)	0.0541	0.0429	0.0655	0.0114	0.0112	0.0113
70(H)	0.0449	0.0397	0.0523	0.0074	0.0052	0.0063
71(H)	0.0537	0.0431	0.0645	0.0107	0.0106	0.0107
72(H)	0.0450	0.0370	0.0448	-0.0002	0.0080	0.0039
73(H)	0.0366	0.0315	0.0389	0.0022	0.0051	0.0037
74(H)	0.0532	0.0352	0.0594	0.0062	0.0180	0.0121
75(H)	0.0439	0.0387	0.0459	0.0020	0.0052	0.0036
76(H)	0.0397	0.0327	0.0424	0.0027	0.0070	0.0048
77(H)	0.0522	0.0375	0.0603	0.0080	0.0148	0.0114
78(H)	0.0257	0.0223	0.0246	-0.0011	0.0034	0.0011
79(H)	0.0205	0.0231	0.0185	-0.0020	-0.0026	-0.0023
80(H)	0.0258	0.0240	0.0279	0.0021	0.0017	0.0019
81(H)	0.0331	0.0305	0.0360	0.0029	0.0026	0.0027
82(H)	0.0471	0.0398	0.0492	0.0021	0.0072	0.0047
83(H)	0.0543	0.0440	0.0593	0.0050	0.0103	0.0076
84(H)	0.0559	0.0407	0.0602	0.0043	0.0152	0.0098
85(H)	0.0304	0.0231	0.0347	0.0043	0.0073	0.0058
86(H)	0.0311	0.0183	0.0373	0.0062	0.0128	0.0095
87(C)	-0.0863	-0.0883	-0.0855	0.0008	0.0020	0.0014
88(H)	0.0351	0.0262	0.0408	0.0057	0.0090	0.0073
89(H)	0.0264	0.0250	0.0272	0.0008	0.0014	0.0011
90(H)	0.0292	0.0265	0.0316	0.0024	0.0027	0.0026
91(H)	0.0287	0.0234	0.0320	0.0033	0.0053	0.0043
92(H)	0.0350	0.0255	0.0412	0.0063	0.0095	0.0079
93(H)	0.0289	0.0295	0.0268	-0.0021	-0.0006	-0.0014
94(H)	0.0241	0.0244	0.0226	-0.0014	-0.0003	-0.0009
95(C)	-0.0418	-0.0447	-0.0372	0.0046	0.0029	0.0038
96(H)	0.0389	0.0316	0.0419	0.0031	0.0073	0.0052
97(C)	-0.0441	-0.0442	-0.0384	0.0057	0.0001	0.0029
98(H)	0.0291	0.0320	0.0363	0.0072	-0.0028	0.0022
99(H)	0.0423	0.0327	0.0469	0.0046	0.0096	0.0071

100(H)	0.0332	0.0327	0.0421	0.0089	0.0005	0.0047
101(C)	-0.0032	0.0043	0.0348	0.0381	-0.0075	0.0153
102(C)	-0.0482	-0.0457	-0.0290	0.0191	-0.0025	0.0083
103(C)	-0.0469	-0.0472	-0.0242	0.0228	0.0003	0.0115
104(C)	-0.0356	-0.0388	-0.0090	0.0266	0.0032	0.0149
105(H)	0.0376	0.0405	0.0513	0.0136	-0.0029	0.0054
106(C)	-0.0374	-0.0419	-0.0084	0.0289	0.0046	0.0168
107(H)	0.0412	0.0411	0.0568	0.0156	0.0001	0.0079
108(C)	0.0020	-0.0049	0.0316	0.0296	0.0069	0.0183
109(H)	0.0454	0.0422	0.0591	0.0136	0.0032	0.0084
110(H)	0.0458	0.0409	0.0628	0.0170	0.0048	0.0109
111(C)	-0.0084	-0.0214	-0.0034	0.0050	0.0130	0.0090
112(H)	0.0433	0.0400	0.0625	0.0191	0.0033	0.0112
113(C)	-0.1391	-0.1522	-0.1234	0.0157	0.0131	0.0144
114(H)	0.0477	0.0412	0.0751	0.0274	0.0065	0.0169
115(H)	0.0412	0.0385	0.0624	0.0212	0.0026	0.0119

[Zr]-H

Condensed local electrophilicity/nucleophilicity index (e*eV)

Atom	Electrophilicity	Nucleophilicity
1(C)	0.10665	0.00985
2(C)	0.09059	0.00639
3(C)	0.02700	0.00366
4(C)	0.11487	0.01621
5(C)	0.03910	0.00289
6(Zr)	1.29771	0.01250
7(C)	0.08619	0.01278
8(C)	0.03523	0.00325
9(C)	0.05287	0.00620
10(C)	0.04867	0.00246
11(C)	0.08574	0.01478
12(Si)	0.04355	0.00353
13(C)	0.03364	0.00333
14(C)	0.03516	0.00340
15(C)	0.09036	0.01478
16(C)	0.05151	0.02323
17(C)	0.12754	0.01861
18(C)	0.15604	0.01454
19(C)	0.04260	0.00354
20(C)	0.03726	0.00358
21(C)	-0.04877	0.00945
22(C)	0.06316	0.01225
23(C)	0.06598	0.01839

24(C)	0.13113	0.01452
25(C)	0.13792	0.01583
26(C)	-0.04532	0.00723
27(C)	0.01015	0.01070
28(C)	0.06175	0.01234
29(C)	0.09835	0.02450
30(C)	0.01228	0.00914
31(C)	0.06232	0.01358
32(C)	-0.02174	0.00556
33(C)	0.05064	0.00952
34(C)	0.10501	0.02104
35(C)	0.04414	0.01015
36(C)	0.08525	0.01289
37(H)	0.08150	0.00695
38(H)	0.07210	0.00693
39(H)	0.06148	0.00620
40(H)	0.01485	0.00118
41(H)	0.05679	0.00477
42(H)	0.05568	0.00521
43(H)	0.06278	0.00576
44(H)	0.01575	0.00134
45(H)	0.05361	0.00904
46(H)	0.09066	0.00980
47(H)	0.10019	0.01033
48(H)	0.06136	0.00787
49(H)	0.09167	0.00847
50(H)	0.09961	0.00997
51(H)	0.00985	0.00575
52(H)	0.05396	0.00934
53(H)	0.06674	0.01161
54(H)	0.00934	0.00549
55(H)	0.05368	0.00928
56(H)	-0.02874	0.00126
57(H)	0.04232	0.00667
58(H)	0.07097	0.01031
59(H)	0.03379	0.00636
60(H)	0.06702	0.00915
61(H)	0.05791	0.00441
62(H)	0.02964	0.00199
63(H)	0.09389	0.00709
64(H)	0.04883	0.00430
65(H)	0.02535	0.00257
66(H)	0.09278	0.00717
67(H)	0.19935	0.00496

Hirshfeld charges, condensed Fukui functions, Units used below are "e" (elementary charge)

Atom	q(N)	q(N+1)	q(N-1)	f-	f+	f0
1(C)	-0.1299	-0.1502	-0.1132	0.0167	0.0203	0.0185
2(C)	0.0155	-0.0017	0.0264	0.0109	0.0172	0.0140
3(C)	-0.0258	-0.0310	-0.0196	0.0062	0.0051	0.0057
4(C)	-0.0496	-0.0714	-0.0220	0.0276	0.0218	0.0247
5(C)	-0.0217	-0.0291	-0.0168	0.0049	0.0074	0.0062
6(Zr)	0.5701	0.3234	0.5914	0.0213	0.2467	0.1340
7(C)	-0.1347	-0.1511	-0.1130	0.0217	0.0164	0.0191
8(C)	-0.0191	-0.0258	-0.0135	0.0055	0.0067	0.0061
9(C)	0.0012	-0.0089	0.0117	0.0105	0.0101	0.0103
10(C)	-0.0090	-0.0182	-0.0048	0.0042	0.0093	0.0067
11(C)	-0.0660	-0.0823	-0.0408	0.0251	0.0163	0.0207
12(Si)	0.3788	0.3706	0.3848	0.0060	0.0083	0.0071
13(C)	-0.1696	-0.1760	-0.1640	0.0057	0.0064	0.0060
14(C)	-0.1701	-0.1768	-0.1643	0.0058	0.0067	0.0062
15(C)	0.0285	0.0113	0.0536	0.0251	0.0172	0.0212
16(C)	-0.0195	-0.0293	0.0200	0.0395	0.0098	0.0246
17(C)	-0.0186	-0.0429	0.0130	0.0316	0.0242	0.0279
18(C)	-0.0124	-0.0421	0.0123	0.0247	0.0297	0.0272
19(C)	-0.0652	-0.0733	-0.0592	0.0060	0.0081	0.0071
20(C)	-0.0686	-0.0757	-0.0625	0.0061	0.0071	0.0066
21(C)	-0.0040	0.0053	0.0121	0.0161	-0.0093	0.0034
22(C)	0.0172	0.0052	0.0380	0.0208	0.0120	0.0164
23(C)	-0.0225	-0.0351	0.0087	0.0313	0.0125	0.0219
24(C)	-0.0239	-0.0488	0.0008	0.0247	0.0249	0.0248
25(C)	-0.0228	-0.0490	0.0041	0.0269	0.0262	0.0266
26(C)	-0.0056	0.0030	0.0067	0.0123	-0.0086	0.0018
27(C)	-0.0391	-0.0410	-0.0209	0.0182	0.0019	0.0101
28(C)	-0.0316	-0.0434	-0.0107	0.0210	0.0117	0.0164
29(C)	-0.0253	-0.0440	0.0164	0.0417	0.0187	0.0302
30(C)	-0.0362	-0.0386	-0.0207	0.0155	0.0023	0.0089
31(C)	-0.0301	-0.0420	-0.0071	0.0231	0.0118	0.0175
32(C)	-0.0406	-0.0364	-0.0311	0.0095	-0.0041	0.0027
33(C)	-0.0302	-0.0399	-0.0140	0.0162	0.0096	0.0129
34(C)	-0.0225	-0.0425	0.0133	0.0358	0.0200	0.0279
35(C)	-0.0328	-0.0412	-0.0155	0.0173	0.0084	0.0128
36(C)	-0.0257	-0.0419	-0.0038	0.0219	0.0162	0.0191
37(H)	0.0652	0.0497	0.0771	0.0118	0.0155	0.0137
38(H)	0.0594	0.0457	0.0712	0.0118	0.0137	0.0127
39(H)	0.0500	0.0383	0.0605	0.0105	0.0117	0.0111
40(H)	0.0385	0.0357	0.0405	0.0020	0.0028	0.0024

41(H)	0.0492	0.0384	0.0573	0.0081	0.0108	0.0095
42(H)	0.0490	0.0384	0.0579	0.0089	0.0106	0.0097
43(H)	0.0501	0.0381	0.0599	0.0098	0.0119	0.0109
44(H)	0.0374	0.0344	0.0397	0.0023	0.0030	0.0026
45(H)	0.0530	0.0428	0.0684	0.0154	0.0102	0.0128
46(H)	0.0572	0.0400	0.0739	0.0167	0.0172	0.0169
47(H)	0.0611	0.0420	0.0786	0.0176	0.0190	0.0183
48(H)	0.0553	0.0436	0.0687	0.0134	0.0117	0.0125
49(H)	0.0567	0.0393	0.0711	0.0144	0.0174	0.0159
50(H)	0.0608	0.0419	0.0778	0.0169	0.0189	0.0179
51(H)	0.0440	0.0421	0.0538	0.0098	0.0019	0.0058
52(H)	0.0536	0.0433	0.0695	0.0159	0.0103	0.0131
53(H)	0.0559	0.0432	0.0757	0.0197	0.0127	0.0162
54(H)	0.0460	0.0443	0.0554	0.0093	0.0018	0.0056
55(H)	0.0543	0.0441	0.0700	0.0158	0.0102	0.0130
56(H)	0.0384	0.0439	0.0406	0.0021	-0.0055	-0.0017
57(H)	0.0539	0.0459	0.0653	0.0113	0.0080	0.0097
58(H)	0.0574	0.0439	0.0749	0.0175	0.0135	0.0155
59(H)	0.0481	0.0416	0.0589	0.0108	0.0064	0.0086
60(H)	0.0569	0.0441	0.0724	0.0156	0.0127	0.0142
61(H)	0.0528	0.0418	0.0603	0.0075	0.0110	0.0093
62(H)	0.0401	0.0345	0.0435	0.0034	0.0056	0.0045
63(H)	0.0541	0.0362	0.0661	0.0121	0.0179	0.0150
64(H)	0.0486	0.0393	0.0559	0.0073	0.0093	0.0083
65(H)	0.0365	0.0317	0.0408	0.0044	0.0048	0.0046
66(H)	0.0562	0.0386	0.0684	0.0122	0.0176	0.0149
67(H)	-0.1781	-0.2160	-0.1697	0.0084	0.0379	0.0232

DVB-PP₁

Condensed local electrophilicity/nucleophilicity index (e*eV)

Atom	Electrophilicity	Nucleophilicity
1(C)	0.00954	0.05736
2(C)	0.08714	0.47297
3(C)	0.05072	0.22136
4(C)	0.00121	0.00729
5(C)	0.05468	0.30856
6(C)	0.02698	0.17169
7(C)	0.03416	0.16473
8(C)	0.03809	0.23827
9(C)	0.03367	0.18262
10(C)	0.03414	0.20573
11(C)	0.00289	0.01659
12(H)	0.00260	0.01801

13(H)	0.00368	0.02074
14(H)	0.00358	0.01892
15(H)	0.02032	0.11273
16(H)	0.01823	0.09279
17(H)	0.02065	0.10929
18(H)	0.02059	0.11522
19(H)	0.01719	0.10329
20(H)	0.00319	0.02149
21(C)	0.00122	0.00749
22(H)	0.00567	0.03191
23(H)	0.00290	0.01653
24(H)	0.00246	0.01408
25(H)	0.00152	0.00956
26(H)	0.00589	0.03320
27(H)	-0.00205	-0.01092
28(H)	0.00226	0.01310
29(C)	0.00270	0.01410
30(H)	0.02457	0.11468
31(C)	0.00188	0.01077
32(H)	0.02863	0.13491
33(H)	0.03557	0.16930
34(H)	0.01493	0.09218

Hirshfeld charges, condensed Fukui functions, Units used below are "e" (elementary charge)

Atom	q(N)	q(N+1)	q(N-1)	f-	f+	f0
1(C)	-0.0441	-0.0597	-0.0267	0.0173	0.0156	0.0165
2(C)	-0.0480	-0.0511	-0.0447	0.0033	0.0031	0.0032
3(C)	-0.0481	-0.0525	-0.0438	0.0043	0.0044	0.0043
4(C)	-0.0119	-0.0139	-0.0097	0.0022	0.0020	0.0021
5(C)	0.0039	-0.0855	0.0971	0.0932	0.0894	0.0913
6(C)	-0.0472	-0.0913	0.0047	0.0519	0.0441	0.0480
7(C)	-0.0397	-0.0955	0.0101	0.0498	0.0559	0.0528
8(C)	-0.0067	-0.0690	0.0653	0.0720	0.0623	0.0671
9(C)	-0.0499	-0.1050	0.0053	0.0552	0.0551	0.0551
10(C)	-0.0430	-0.0989	0.0191	0.0621	0.0558	0.0590
11(C)	-0.0874	-0.0922	-0.0824	0.0050	0.0047	0.0049
12(H)	0.0275	0.0233	0.0330	0.0054	0.0042	0.0048
13(H)	0.0249	0.0189	0.0311	0.0063	0.0060	0.0061
14(H)	0.0255	0.0196	0.0312	0.0057	0.0059	0.0058
15(H)	0.0399	0.0066	0.0739	0.0340	0.0332	0.0336
16(H)	0.0415	0.0117	0.0695	0.0280	0.0298	0.0289
17(H)	0.0387	0.0049	0.0717	0.0330	0.0338	0.0334
18(H)	0.0397	0.0061	0.0745	0.0348	0.0337	0.0342
19(H)	0.0330	0.0049	0.0642	0.0312	0.0281	0.0297

20(H)	0.0271	0.0219	0.0336	0.0065	0.0052	0.0059
21(C)	-0.0880	-0.0899	-0.0857	0.0023	0.0020	0.0021
22(H)	0.0285	0.0192	0.0381	0.0096	0.0093	0.0095
23(H)	0.0274	0.0226	0.0324	0.0050	0.0047	0.0049
24(H)	0.0281	0.0241	0.0324	0.0043	0.0040	0.0041
25(H)	0.0249	0.0224	0.0278	0.0029	0.0025	0.0027
26(H)	0.0289	0.0193	0.0389	0.0100	0.0096	0.0098
27(H)	0.0281	0.0315	0.0248	-0.0033	-0.0033	-0.0033
28(H)	0.0274	0.0237	0.0313	0.0040	0.0037	0.0038
29(C)	-0.0402	-0.1231	0.0267	0.0669	0.0830	0.0749
30(H)	0.0392	-0.0010	0.0738	0.0346	0.0402	0.0374
31(C)	-0.0908	-0.2333	0.0520	0.1429	0.1425	0.1427
32(H)	0.0377	-0.0091	0.0785	0.0408	0.0468	0.0438
33(H)	0.0405	-0.0176	0.0917	0.0511	0.0582	0.0547
34(H)	0.0326	0.0082	0.0605	0.0278	0.0244	0.0261

[BVPE]-PP₁

Condensed local electrophilicity/nucleophilicity index (e*eV)

Atom	Electrophilicity	Nucleophilicity
1(C)	0.00329	0.03158
2(C)	0.07020	0.30817
3(C)	0.03883	0.13969
4(C)	0.00066	0.00856
5(C)	0.03866	0.16628
6(C)	0.02143	0.09673
7(C)	0.02538	0.11593
8(C)	0.03084	0.14698
9(C)	0.02379	0.10096
10(C)	0.02880	0.12119
11(C)	0.00186	0.01542
12(H)	0.00055	0.01263
13(H)	0.00219	0.01715
14(H)	0.00234	0.01688
15(H)	0.01570	0.06820
16(H)	0.01456	0.06461
17(H)	0.01435	0.05876
18(H)	0.01709	0.07469
19(H)	0.00603	0.04564
20(H)	0.00146	0.01574
21(C)	0.00053	0.00500
22(H)	0.00347	0.02508
23(H)	0.00187	0.01337
24(H)	0.00171	0.01221

25(H)	0.00070	0.00730
26(H)	0.00344	0.02317
27(H)	-0.00178	-0.00760
28(H)	0.00119	0.00910
29(C)	0.00170	0.01681
30(H)	0.01930	0.07549
31(C)	0.00184	0.02803
32(H)	0.02282	0.08839
33(H)	0.02878	0.11440
34(H)	0.00593	0.04354
35(C)	0.00828	0.03109
36(H)	0.01231	0.04726
37(H)	0.01219	0.04719
38(C)	0.00425	0.02817
39(H)	0.00586	0.04068
40(H)	0.00588	0.04121
41(C)	0.00808	0.14198
42(C)	0.02566	0.09118
43(C)	0.00949	0.08445
44(C)	0.01634	0.11178
45(H)	0.01180	0.05827
46(C)	0.02777	0.10392
47(H)	0.00568	0.04498
48(C)	0.01857	0.17456
49(H)	0.01162	0.07026
50(H)	0.01402	0.06691

Hirshfeld charges, condensed Fukui functions, Units used below are "e" (elementary charge)

Atom	q(N)	q(N+1)	q(N-1)	f-	f+	f0
1(C)	-0.0460	-0.0511	-0.0363	0.0097	0.0051	0.0074
2(C)	-0.0899	-0.1984	0.0045	0.0944	0.1084	0.1014
3(C)	-0.0400	-0.1000	0.0028	0.0428	0.0600	0.0514
4(C)	-0.0118	-0.0128	-0.0092	0.0026	0.0010	0.0018
5(C)	0.0043	-0.0554	0.0552	0.0509	0.0597	0.0553
6(C)	-0.0466	-0.0797	-0.0169	0.0296	0.0331	0.0314
7(C)	-0.0390	-0.0782	-0.0035	0.0355	0.0392	0.0374
8(C)	-0.0060	-0.0536	0.0391	0.0450	0.0476	0.0463
9(C)	-0.0498	-0.0865	-0.0188	0.0309	0.0368	0.0338
10(C)	-0.0426	-0.0871	-0.0055	0.0371	0.0445	0.0408
11(C)	-0.0877	-0.0906	-0.0830	0.0047	0.0029	0.0038
12(H)	0.0264	0.0255	0.0303	0.0039	0.0008	0.0024
13(H)	0.0242	0.0208	0.0295	0.0053	0.0034	0.0043
14(H)	0.0249	0.0213	0.0301	0.0052	0.0036	0.0044
15(H)	0.0404	0.0161	0.0613	0.0209	0.0243	0.0226

16(H)	0.0420	0.0195	0.0618	0.0198	0.0225	0.0211
17(H)	0.0387	0.0165	0.0567	0.0180	0.0222	0.0201
18(H)	0.0402	0.0138	0.0630	0.0229	0.0264	0.0246
19(H)	0.0298	0.0205	0.0438	0.0140	0.0093	0.0117
20(H)	0.0260	0.0237	0.0308	0.0048	0.0023	0.0035
21(C)	-0.0880	-0.0888	-0.0865	0.0015	0.0008	0.0012
22(H)	0.0282	0.0228	0.0359	0.0077	0.0054	0.0065
23(H)	0.0271	0.0242	0.0312	0.0041	0.0029	0.0035
24(H)	0.0279	0.0252	0.0316	0.0037	0.0026	0.0032
25(H)	0.0249	0.0239	0.0272	0.0022	0.0011	0.0017
26(H)	0.0286	0.0233	0.0357	0.0071	0.0053	0.0062
27(H)	0.0287	0.0315	0.0264	-0.0023	-0.0027	-0.0025
28(H)	0.0268	0.0250	0.0296	0.0028	0.0018	0.0023
29(C)	-0.0492	-0.0519	-0.0441	0.0052	0.0026	0.0039
30(H)	0.0395	0.0097	0.0626	0.0231	0.0298	0.0265
31(C)	-0.0482	-0.0510	-0.0396	0.0086	0.0028	0.0057
32(H)	0.0380	0.0028	0.0651	0.0271	0.0353	0.0312
33(H)	0.0410	-0.0035	0.0760	0.0350	0.0445	0.0398
34(H)	0.0301	0.0210	0.0435	0.0133	0.0092	0.0113
35(C)	-0.0431	-0.0559	-0.0336	0.0095	0.0128	0.0112
36(H)	0.0349	0.0159	0.0494	0.0145	0.0190	0.0168
37(H)	0.0349	0.0161	0.0493	0.0145	0.0188	0.0166
38(C)	-0.0435	-0.0501	-0.0349	0.0086	0.0066	0.0076
39(H)	0.0340	0.0250	0.0465	0.0125	0.0090	0.0108
40(H)	0.0341	0.0250	0.0467	0.0126	0.0091	0.0109
41(C)	-0.0010	-0.0135	0.0425	0.0435	0.0125	0.0280
42(C)	-0.0492	-0.0889	-0.0213	0.0279	0.0396	0.0338
43(C)	-0.0510	-0.0657	-0.0251	0.0259	0.0147	0.0203
44(C)	-0.0477	-0.0730	-0.0135	0.0342	0.0252	0.0297
45(H)	0.0390	0.0207	0.0568	0.0179	0.0182	0.0180
46(C)	-0.0488	-0.0917	-0.0170	0.0318	0.0429	0.0374
47(H)	0.0370	0.0283	0.0508	0.0138	0.0088	0.0113
48(C)	0.0002	-0.0285	0.0536	0.0535	0.0287	0.0411
49(H)	0.0389	0.0210	0.0605	0.0215	0.0180	0.0197
50(H)	0.0383	0.0166	0.0588	0.0205	0.0217	0.0211

Table S2: Energies and Cartesian coordinates of all the structures for the main text.

Gibbs free energies (G) and enthalpies (H) (in *a.u.*) of all the structures for the main text

	[Zr]-DVB-PP₁	H₂	TS1	IM1	TS2
G	-2193.359353	-1.171228	-2194.515816	-2194.513368	-2194.508915
H	-2193.225599	-1.156436	-2194.37978	-2194.379866	-2194.377058
	IM2	DVB-PP₁	[Zr]-H	[Zr]-BVPE-PP₁	[TS1]
G	-2194.542299	-544.972075	-1649.56962	-2502.746674	-2503.899192
H	-2194.405323	-544.911639	-1649.472072	-2502.594457	-2503.746689
	[IM1]	[TS2]	[IM2]	BVPE-PP₁	
G	-2503.901661	-2503.898058	-2503.927253	-854.3605529	
H	-2503.748013	-2503.744805	-2503.771216	-854.2799269	
	IM3_{1,2}	TS3_{1,2}	PR3_{1,2}	IM3_{2,1}	TS3_{2,1}
G	-2194.546812	-2194.542051	-2194.56112	-2194.536863	-2194.534211
H	-2194.410721	-2194.406035	-2194.426021	-2194.404326	-2194.402761
	PR3_{2,1}	[IM3_{1,2}]	[TS3_{1,2}]	[PR3_{1,2}]	[IM3_{2,1}]
G	-2194.55063	-2503.934614	-2503.922543	-2503.950246	-2503.923243
H	-2194.418368	-2503.778545	-2503.768083	-2503.796347	-2503.770393
	[TS3_{2,1}]	[PR3_{2,1}]			
G	-2503.918592	-2503.938919			
H	-2503.767999	-2503.787615			

[Zr]-DVB-PP₁

C	-0.18666300	1.51375100	0.75731400
C	0.83383800	-2.28992200	-1.63438300
C	1.13220500	-2.62891500	-0.26667200
C	1.60018900	-1.07766100	-1.91247900
C	1.98750200	-1.64448800	0.28861400
C	2.36809000	-0.71491000	-0.73488700
Zr	-0.36705800	-0.59548600	-0.34121100
C	-1.81795200	-1.55025700	-2.12126400

C	-2.61294600	-1.59008400	-0.90407300
C	-1.76967300	-0.15587000	-2.50397800
C	-3.00864600	-0.23637200	-0.55536100
C	-2.40513400	0.63162000	-1.51695800
Si	-0.61404800	-2.90603600	-2.70299800
C	-1.17466300	-4.65892500	-2.28845300
C	-0.26917500	-2.95540900	-4.55580500
C	-3.88684200	0.02418300	0.54778900
C	-3.01488300	-2.65956900	-0.05236300
C	-4.27638100	-1.06991800	1.31286800
C	-3.83553900	-2.38480500	1.02648400
C	0.67454000	-3.84005600	0.51038000
C	-1.32029200	0.44474000	-3.81192100
C	-4.37537000	1.38985900	0.86207600
C	3.41601700	0.26973600	-0.82491400
C	1.76642600	-0.32988100	-3.11210500
C	3.49820200	0.97862900	-2.01662400
C	2.67661100	0.70190300	-3.13430800
C	4.49450000	0.42828700	0.18731400
C	-4.87278700	2.23538700	-0.14601800
C	-5.35992500	3.50337200	0.16720700
C	-5.35176000	3.95350400	1.48932600
C	-4.38569100	1.85023200	2.19113300
C	-4.86472500	3.12260700	2.50021500
C	4.27395900	0.34624200	1.57101900
C	5.32132000	0.49876600	2.47941800
C	6.62049400	0.72716200	2.02602100
C	5.81588100	0.64408100	-0.25353700
C	6.86250100	0.79545200	0.65275500
C	0.74136500	2.69539500	0.50879900
C	0.41153400	3.44623900	-0.79133900
C	1.09458100	4.81994300	-0.94255100
C	-0.00363700	0.67299800	1.93483300
C	-0.88964900	-0.43599400	2.14344300
C	-0.63440200	-1.41319700	3.12839700
C	0.47658400	-1.32660700	3.96609800
C	1.09316100	0.76655200	2.83250500
C	1.29987600	-0.17963500	3.81910300
C	0.57592200	5.54075400	-2.19555000
H	2.37986400	-1.68605200	1.29450900
H	-2.52751800	1.70423800	-1.56933200
H	-0.42856400	-5.36213200	-2.67556300
H	-1.31423900	-4.88644300	-1.23173800
H	-2.11654000	-4.86949600	-2.80755800

H	0.43793900	-3.76964000	-4.75137000
H	-1.19827100	-3.19578200	-5.08515800
H	0.14454500	-2.05387100	-5.00801000
H	-2.75505200	-3.68321500	-0.29079500
H	-4.96810000	-0.91586400	2.13490300
H	-4.19053200	-3.20185800	1.64750400
H	1.23559800	-0.60537100	-4.01098000
H	4.25488800	1.74940900	-2.11340100
H	2.82073800	1.27405200	-4.04581800
H	-4.91529300	1.88267900	-1.17182700
H	-5.75619800	4.13658600	-0.62083100
H	-5.72836600	4.94265400	1.73068100
H	-4.00252700	1.21292500	2.98305100
H	-4.85725300	3.46440800	3.53072000
H	3.27267300	0.18906400	1.94422200
H	5.12087900	0.44103100	3.54563800
H	7.43638000	0.84171500	2.73291000
H	6.03104500	0.66046700	-1.31693400
H	7.87137400	0.95400600	0.28404300
H	1.05274300	-3.79862600	1.53425000
H	-0.41300200	-3.94034700	0.56283400
H	1.06092300	-4.75187300	0.04320000
H	-0.65364300	1.30018400	-3.67229900
H	-0.83338900	-0.27586000	-4.46398800
H	-2.20831900	0.80715000	-4.34246400
H	1.78477100	2.36326500	0.49076800
H	0.67418600	2.81542900	-1.65418000
H	-0.67585600	3.60120000	-0.83929200
H	-1.90672300	-0.39023900	1.75614800
H	-1.36080200	-2.20794000	3.26646400
H	1.75240800	1.62463400	2.76788600
H	2.12867300	-0.04583600	4.51036300
H	-1.23565800	1.79734700	0.62992900
H	0.65764300	3.40431800	1.34869000
C	2.62723000	4.72313100	-0.96911000
H	1.01452400	6.53939300	-2.28817800
H	0.83353900	4.98276700	-3.10464100
H	-0.51334900	5.65630300	-2.17118200
H	0.81015300	5.42308600	-0.06708000
H	3.07732400	5.71564300	-1.07279200
H	3.03163600	4.27402000	-0.05664300
H	2.96389400	4.11755300	-1.81963600
C	0.79613400	-2.31729400	5.00519700
H	1.56609900	-2.00928900	5.71092300

C	0.25335000	-3.53334700	5.14688800
H	-0.50734200	-3.92109400	4.47475400
H	0.55945100	-4.18923800	5.95446000

TS1

C	-0.44802600	1.56375600	0.59197900
C	1.27237400	-2.57515900	-1.07921300
C	1.55178100	-2.42844000	0.32418700
C	1.94035000	-1.45810400	-1.73369600
C	2.25886700	-1.21103600	0.53957900
C	2.57825500	-0.62643300	-0.73117000
Zr	-0.15351500	-0.67899700	-0.28424400
C	-1.44236800	-2.27003500	-1.67034400
C	-2.28575900	-2.09803900	-0.49867400
C	-1.55134700	-1.03099900	-2.41236700
C	-2.85973100	-0.76601700	-0.52229800
C	-2.32763400	-0.10665400	-1.67414800
Si	-0.10333800	-3.59925800	-1.90611000
C	-0.45224600	-5.23173000	-1.03124600
C	0.20226000	-4.04400000	-3.71187600
C	-3.81126300	-0.34731500	0.46222400
C	-2.62444700	-2.97621500	0.57070100
C	-4.12026700	-1.26144600	1.46380800
C	-3.53263700	-2.54970300	1.52013300
C	1.24700300	-3.41853100	1.42345900
C	-1.11672400	-0.74076000	-3.82725300
C	-4.46436300	0.98543500	0.41672900
C	3.51798400	0.39335400	-1.12592600
C	2.20004900	-1.22556300	-3.11437100
C	3.69124100	0.59259900	-2.48761300
C	3.04592700	-0.20160700	-3.46910100
C	4.40891900	1.09722000	-0.16885800
C	-5.01169500	1.48905700	-0.77696600
C	-5.64914700	2.72876000	-0.79866200
C	-5.74641100	3.49029600	0.36809100
C	-4.58122200	1.75614700	1.58739100
C	-5.21217800	2.99941300	1.56110000
C	3.94145500	1.61632300	1.04640700
C	4.79729900	2.28639000	1.91984000
C	6.14616800	2.44299900	1.59809500
C	5.77337300	1.25541700	-0.47700100
C	6.63060900	1.92171900	0.39656700
C	0.19673400	2.90097100	0.22356700

C	-0.67880800	3.74067200	-0.72056100
C	-0.13256900	5.14739100	-1.03715500
C	-0.11669300	0.90103600	1.83898900
C	-0.79220300	-0.32302300	2.16729100
C	-0.39883800	-1.10751700	3.27559200
C	0.66009400	-0.73079100	4.09541200
C	0.92983400	1.29086400	2.72288600
C	1.28073100	0.51684700	3.80926100
C	-1.17959800	5.96381300	-1.80948400
H	0.97666700	1.30680400	-2.68521900
H	0.35092700	1.60437200	-2.41389400
H	2.62775000	-0.87836700	1.49982300
H	-2.58599900	0.88780000	-2.00999800
H	0.34287600	-5.93916300	-1.29361700
H	-0.49595300	-5.18554100	0.05712800
H	-1.39468000	-5.65604100	-1.39500600
H	1.16389200	-4.55834700	-3.81746200
H	-0.57842100	-4.74612500	-4.02654700
H	0.18354400	-3.20771100	-4.41160200
H	-2.23899400	-3.98799500	0.59992100
H	-4.86602400	-0.99365000	2.20547700
H	-3.83777900	-3.22806700	2.31126000
H	1.80814600	-1.89537700	-3.86835800
H	4.38935200	1.35527000	-2.81669500
H	3.27212000	-0.02550700	-4.51642400
H	-4.97318400	0.89042700	-1.68182000
H	-6.08010400	3.09519900	-1.72548200
H	-6.24167100	4.45617700	0.34905200
H	-4.16220600	1.38507100	2.51846800
H	-5.28673400	3.58396200	2.47306200
H	2.89488000	1.51317600	1.29529100
H	4.41043900	2.69207600	2.85065500
H	6.81483000	2.96155600	2.27821900
H	6.16894000	0.82951400	-1.39378700
H	7.68102000	2.02577100	0.14217600
H	1.59620000	-3.04161200	2.38608600
H	0.18275500	-3.64911900	1.52318900
H	1.76621300	-4.36087500	1.21967900
H	-1.34949100	0.29465500	-4.08665600
H	-0.05488000	-0.89290000	-4.01173600
H	-1.67416200	-1.38756900	-4.51340100
H	1.19117600	2.75348100	-0.21238700
H	-0.83863300	3.20219300	-1.66671900
H	-1.67177900	3.84661200	-0.26257600

H	-1.80120300	-0.48315400	1.79475900
H	-0.98284200	-1.99155000	3.51111800
H	1.41618100	2.24759200	2.57284500
H	2.05868500	0.87291400	4.48039700
H	-1.52903500	1.57775800	0.42757500
H	0.35570300	3.49533300	1.13609700
C	1.19671400	5.10868700	-1.80702900
H	-0.82453900	6.98146500	-2.00052600
H	-1.39768800	5.50290000	-2.78094300
H	-2.12151900	6.03614500	-1.25512700
H	0.04679900	5.65468300	-0.07700000
H	1.55125600	6.12237100	-2.01967000
H	1.98782300	4.59761400	-1.24917900
H	1.07554300	4.59421600	-2.76860400
C	1.12290000	-1.51775000	5.24855700
H	1.81101300	-0.99706600	5.91279200
C	0.79878900	-2.78528700	5.53609100
H	1.19550300	-3.27539100	6.41841900
H	0.13339900	-3.37854600	4.91471300

IM1

C	-0.39850100	1.67025400	0.62054900
C	1.09484500	-2.67606400	-1.03837400
C	1.36508000	-2.51520400	0.36676600
C	1.83277100	-1.61914700	-1.70869400
C	2.17460200	-1.35853600	0.55813200
C	2.53244000	-0.81857800	-0.71580500
Zr	-0.15807600	-0.61629000	-0.37882300
C	-1.58972300	-2.21184000	-1.63192500
C	-2.39961600	-1.97164800	-0.44652600
C	-1.65504000	-0.99079100	-2.40325300
C	-2.92323900	-0.62111200	-0.50051000
C	-2.38246700	-0.01539000	-1.67273100
Si	-0.34042300	-3.62827700	-1.84637100
C	-0.78582300	-5.22294800	-0.94619700
C	-0.05979300	-4.12891800	-3.64228600
C	-3.84854200	-0.13919900	0.48178800
C	-2.78240700	-2.81758700	0.63569100
C	-4.19410800	-1.01824400	1.49834600
C	-3.66595000	-2.33425500	1.57669400
C	1.00871000	-3.47058500	1.48041300
C	-1.23981600	-0.75113500	-3.83361700
C	-4.43919700	1.22269500	0.41320500

C	3.50734000	0.16337700	-1.13228600
C	2.07198600	-1.38866700	-3.09804900
C	3.64102300	0.37090500	-2.49638700
C	2.94009400	-0.39130900	-3.46711300
C	4.45755100	0.82174900	-0.19945000
C	-4.98147600	1.72387100	-0.78368600
C	-5.56287000	2.99054100	-0.82546800
C	-5.60956900	3.78166400	0.32452600
C	-4.50327500	2.02491700	1.56647400
C	-5.08006700	3.29395200	1.52081200
C	4.07189800	1.29622400	1.06305700
C	4.98718000	1.92350600	1.90780000
C	6.31565000	2.08177200	1.51161900
C	5.80470300	0.97735700	-0.57955500
C	6.72044100	1.60194100	0.26437500
C	0.28557300	3.00463300	0.33656000
C	-0.29442900	3.75680400	-0.87180300
C	0.25244400	5.18607500	-1.06522900
C	-0.07373200	0.93906500	1.82459800
C	-0.80013800	-0.25193800	2.14708500
C	-0.44531400	-1.04753300	3.25868300
C	0.62734300	-0.71641800	4.07923800
C	1.00258000	1.27954600	2.69745400
C	1.31748800	0.49339900	3.78341700
C	-0.53386900	5.91217500	-2.16659400
H	0.48998200	0.63849300	-1.93646500
H	0.32415500	1.15039400	-1.36713100
H	2.55403200	-1.03437300	1.51652300
H	-2.60051500	0.98190400	-2.02971100
H	-0.04282900	-5.98351100	-1.21275100
H	-0.80908600	-5.16235700	0.14182500
H	-1.75962700	-5.58757800	-1.29139900
H	0.87728200	-4.68905500	-3.73534400
H	-0.87161500	-4.80322000	-3.93840400
H	-0.04219000	-3.31238500	-4.36490200
H	-2.44254400	-3.84459700	0.68376900
H	-4.92404700	-0.70409000	2.23780200
H	-4.00172500	-2.98302900	2.38012200
H	1.63439300	-2.03752800	-3.84515100
H	4.35352400	1.11249700	-2.84195500
H	3.14256300	-0.21193100	-4.51863000
H	-4.98429400	1.10351600	-1.67468400
H	-5.99093400	3.35483700	-1.75455500
H	-6.06185300	4.76799900	0.29006200

H	-4.08766600	1.65565200	2.49985100
H	-5.11566300	3.90110200	2.42034000
H	3.04402700	1.19077900	1.37989200
H	4.66188000	2.29239700	2.87664000
H	7.02998000	2.56665200	2.16975300
H	6.14312700	0.57929100	-1.53082900
H	7.75508500	1.70369300	-0.04877900
H	1.37674900	-3.09761500	2.43742500
H	-0.06559700	-3.64265900	1.58252800
H	1.48089500	-4.44089500	1.29426000
H	-1.28235000	0.31620000	-4.06870400
H	-0.23895900	-1.10360700	-4.07318300
H	-1.94215400	-1.26173400	-4.50237300
H	1.36637000	2.86735900	0.21286800
H	-0.11470300	3.19107200	-1.79914100
H	-1.38531300	3.81266400	-0.75490700
H	-1.80190300	-0.38305800	1.75268500
H	-1.06864700	-1.90405500	3.49354400
H	1.53629800	2.20930700	2.53923800
H	2.11468100	0.81019700	4.45165100
H	-1.47301900	1.70502500	0.42713600
H	0.16526900	3.65147000	1.22023700
C	1.75768100	5.20513700	-1.37220300
H	-0.18947000	6.94465600	-2.28195400
H	-0.40636200	5.41251500	-3.13504400
H	-1.60576500	5.94023400	-1.94289500
H	0.09071000	5.72997900	-0.12252900
H	2.11269600	6.23131400	-1.51030300
H	2.35443900	4.76009100	-0.56975200
H	1.97401800	4.65575800	-2.29747900
C	1.04689400	-1.51247300	5.24251400
H	1.79212100	-1.03607500	5.87774300
C	0.62187000	-2.73886100	5.57400800
H	0.99847500	-3.23739800	6.46042400
H	-0.11029300	-3.28788100	4.98840300

TS2

C	-0.40167500	1.74463700	0.54979800
C	1.10132800	-2.75822100	-0.92601600
C	1.35844000	-2.52433900	0.47247600
C	1.86105000	-1.74788600	-1.64539500
C	2.16816300	-1.35977900	0.60876400
C	2.54821800	-0.89722800	-0.69131400
Zr	-0.14011500	-0.67490600	-0.36733600

C	-1.57204900	-2.29800900	-1.56292200
C	-2.39537600	-1.99992900	-0.39829900
C	-1.62094900	-1.11190400	-2.39071300
C	-2.90548100	-0.64956900	-0.51761400
C	-2.34802600	-0.10274500	-1.71211500
Si	-0.33461700	-3.73474900	-1.70263800
C	-0.79988300	-5.28379000	-0.73537700
C	-0.05059200	-4.31234800	-3.47446800
C	-3.84052200	-0.11828100	0.43019000
C	-2.79977500	-2.79523300	0.71313500
C	-4.20886900	-0.95030300	1.47777600
C	-3.69294900	-2.26572600	1.61990100
C	0.98900200	-3.41688700	1.63283500
C	-1.17071900	-0.93243800	-3.81794600
C	-4.41499300	1.24596000	0.29714100
C	3.53113600	0.05569700	-1.14707500
C	2.12585000	-1.60477900	-3.03913800
C	3.70417000	0.17004900	-2.51762100
C	3.01774600	-0.64577100	-3.45218600
C	4.44695000	0.78433100	-0.23303900
C	-4.93234900	1.70559600	-0.92721200
C	-5.49827500	2.97600800	-1.02828000
C	-5.55416000	3.81267500	0.08859100
C	-4.48818200	2.09440100	1.41653700
C	-5.04964300	3.36685700	1.31171800
C	4.00259900	1.37676600	0.95784700
C	4.88004900	2.07496400	1.78687600
C	6.22862400	2.18701900	1.44590600
C	5.81184400	0.89663400	-0.55834100
C	6.69067800	1.59105800	0.27072300
C	0.25738200	3.10219800	0.29114000
C	-0.27431800	3.81234600	-0.96351600
C	0.27050700	5.24037900	-1.17134200
C	-0.08205000	1.03074800	1.78988200
C	-0.82805100	-0.12940100	2.15355700
C	-0.50565900	-0.87724400	3.30234600
C	0.55819100	-0.51927800	4.12813900
C	0.97670000	1.40341800	2.66066200
C	1.26781500	0.66241000	3.78885800
C	-0.47607400	5.93120300	-2.32193600
H	0.39279700	0.69969400	-1.61211300
H	0.15132300	1.19467200	-0.86300500
H	2.54450500	-0.98644800	1.55092300
H	-2.54799200	0.88094100	-2.11452100

H	-0.05832100	-6.05925000	-0.95985200
H	-0.83373800	-5.17452700	0.34888500
H	-1.77217500	-5.65895100	-1.07353300
H	0.88387400	-4.88005100	-3.54405700
H	-0.86556600	-4.99393700	-3.74426500
H	-0.02903300	-3.52409900	-4.22786200
H	-2.46761800	-3.82138500	0.80933700
H	-4.94673200	-0.59910500	2.19237100
H	-4.04605900	-2.87739200	2.44474500
H	1.69199000	-2.29162100	-3.75385200
H	4.43126900	0.88350600	-2.89154200
H	3.24425600	-0.53639000	-4.50837300
H	-4.92825900	1.05058700	-1.79296500
H	-5.90719700	3.30787200	-1.97790700
H	-5.99448300	4.80171300	0.00780000
H	-4.09333600	1.75742100	2.37096700
H	-5.09321000	4.00922500	2.18611800
H	2.95776500	1.30479300	1.22635900
H	4.51080100	2.53595000	2.69900600
H	6.91402400	2.72726700	2.09156300
H	6.19066600	0.41336600	-1.45342800
H	7.74067100	1.65839400	0.00255500
H	1.31983600	-2.97731400	2.57536300
H	-0.08329900	-3.61066800	1.71370500
H	1.48917700	-4.38505500	1.52248200
H	-1.22018200	0.12272200	-4.09987500
H	-0.15664000	-1.27615100	-4.00949900
H	-1.84477300	-1.48524500	-4.48237000
H	1.34575800	2.98975400	0.22556300
H	-0.04377800	3.21707300	-1.86009800
H	-1.36986700	3.86088300	-0.89812300
H	-1.80572600	-0.29391600	1.71326000
H	-1.14037100	-1.71857600	3.55974300
H	1.52861300	2.31561400	2.46848400
H	2.06207000	0.99884400	4.45060200
H	-1.47832500	1.77904000	0.36651700
H	0.06758800	3.74672200	1.16273600
C	1.78660300	5.26231200	-1.41991600
H	-0.13114500	6.96157200	-2.45314200
H	-0.30973700	5.40462700	-3.26985800
H	-1.55580500	5.96047700	-2.14005600
H	0.06787200	5.80747000	-0.25030300
H	2.13993000	6.28741200	-1.56963500
H	2.35559900	4.84200600	-0.58448500

H	2.04219500	4.69138000	-2.32159000
C	0.94774900	-1.26813000	5.33301500
H	1.69870100	-0.77977800	5.95199200
C	0.48810900	-2.46575100	5.71787400
H	-0.25283400	-3.02341600	5.15187700
H	0.84447500	-2.93117800	6.63028300

IM2

C	2.43117800	2.23349200	-0.15361500
C	-1.66868000	-2.92996600	-0.24906400
C	-1.26825900	-2.65521600	1.10834200
C	-0.43589500	-2.97307400	-1.02435900
C	0.13457100	-2.43152200	1.14675000
C	0.68627800	-2.68817900	-0.15393300
Zr	-0.96942300	-0.57381800	-0.26105500
C	-3.20921000	-0.83866500	-1.25848300
C	-3.44812100	0.15939100	-0.22579900
C	-2.45245300	-0.15830900	-2.28925900
C	-2.80772900	1.40006200	-0.61281000
C	-2.14568200	1.15193300	-1.85674200
Si	-3.39701400	-2.71623100	-1.01489300
C	-4.80320500	-3.22940300	0.13155100
C	-3.68854700	-3.66182100	-2.61880900
C	-2.97772100	2.59891200	0.16025100
C	-4.22108900	0.12549200	0.97149300
C	-3.75480300	2.50123000	1.30487300
C	-4.36470000	1.28352800	1.70596100
C	-2.12910400	-2.66211400	2.34675200
C	-2.10320700	-0.63792000	-3.67360500
C	-2.39221000	3.89982900	-0.25439400
C	2.03403800	-2.84234000	-0.62695600
C	-0.19978400	-3.31913300	-2.38225900
C	2.19240600	-3.17326900	-1.96670100
C	1.09938800	-3.39975700	-2.83312100
C	3.21736600	-2.80486700	0.26828300
C	-2.49632000	4.36136500	-1.57927200
C	-1.97437800	5.60195600	-1.94351300
C	-1.33476500	6.40299400	-0.99514100
C	-1.75570000	4.72242400	0.69276300
C	-1.22939800	5.96015800	0.32486000
C	3.36595900	-1.84102600	1.27742200
C	4.49375000	-1.83019500	2.09832900
C	5.49483700	-2.78850700	1.93327300
C	4.23239000	-3.76817600	0.11708000

C	5.35776800	-3.75870300	0.93863600
C	3.96067600	2.15153500	-0.07847800
C	4.62923500	2.68510100	-1.35340800
C	6.17078200	2.70673700	-1.31902200
C	1.66580500	1.68185700	1.03319500
C	0.25702100	1.58973400	0.97667100
C	-0.50335100	1.11281000	2.05683700
C	0.12413900	0.72317400	3.26453300
C	2.27177700	1.30422000	2.23634400
C	1.52151300	0.83422100	3.31720200
C	6.72119000	3.43732700	-2.55287800
H	0.29918800	-0.23555200	-1.51857100
H	2.08492700	1.70913200	-1.05398700
H	0.70077000	-2.24530400	2.04932600
H	-1.58781600	1.87184900	-2.43887000
H	-4.87958900	-4.32265000	0.10710300
H	-4.69723000	-2.93749000	1.17661200
H	-5.75283000	-2.83049900	-0.24217400
H	-3.47154600	-4.72602100	-2.47454400
H	-4.75148400	-3.57846900	-2.87320300
H	-3.12330200	-3.31194800	-3.48319300
H	-4.75499800	-0.77145100	1.25893400
H	-3.94449700	3.39721100	1.88751600
H	-4.99738800	1.28253500	2.58860400
H	-1.02049700	-3.59355600	-3.03206000
H	3.19746100	-3.28702600	-2.35948300
H	1.29594100	-3.68439900	-3.86222700
H	-3.02520700	3.76644100	-2.31714800
H	-2.07877600	5.94859700	-2.96722400
H	-0.92837700	7.36815500	-1.28126000
H	-1.66382600	4.38255200	1.72032200
H	-0.73815700	6.57872000	1.06995900
H	2.61042800	-1.07624800	1.40154100
H	4.59273000	-1.06998900	2.86824700
H	6.37022800	-2.78277800	2.57533100
H	4.12432900	-4.54708300	-0.63128800
H	6.12391100	-4.51690100	0.80800500
H	-1.55564100	-2.33366700	3.21561500
H	-3.00702000	-2.01709800	2.27161300
H	-2.48570300	-3.67945700	2.54167000
H	-1.38192300	0.03943500	-4.13690700
H	-1.67582500	-1.63843500	-3.69910300
H	-3.00750700	-0.64466900	-4.29332700
H	4.25801700	1.11032600	0.09433800

H	4.29921300	2.08566600	-2.21494200
H	4.26870700	3.70670700	-1.53751400
H	-0.24719300	2.03158800	0.11771400
H	-1.58927200	1.16975600	2.01242800
H	3.34801200	1.38216100	2.34238300
H	2.03452100	0.56455700	4.23663400
H	2.13073000	3.28258500	-0.29072500
H	4.32287300	2.73119300	0.78154900
C	6.77724000	1.29907800	-1.21019200
H	7.81381000	3.49758400	-2.52185400
H	6.44514700	2.91188400	-3.47522900
H	6.33158900	4.45876700	-2.62186400
H	6.47432500	3.27729500	-0.42799900
H	7.87086600	1.34779000	-1.19680500
H	6.46226200	0.77663200	-0.30133300
H	6.48484500	0.68197900	-2.06899000
C	-0.60135500	0.28521900	4.46665100
H	0.03700500	-0.07144700	5.27339100
C	-1.92469900	0.31969700	4.67192800
H	-2.62811900	0.68674600	3.93058300
H	-2.34664700	-0.01364100	5.61412000

DVB-PP₁

C	0.67016600	-1.05176400	-0.00549600
C	1.78293900	-0.00460400	-0.12699800
C	3.18169000	-0.63105000	-0.04922600
C	4.35311600	0.34814800	-0.26164600
C	-0.75869800	-0.53697500	-0.02330000
C	-1.81174300	-1.43144700	0.23916800
C	-3.13716300	-1.02149400	0.22468600
C	-3.47822300	0.31603500	-0.05367200
C	-1.09528400	0.79154500	-0.29903400
C	-2.42751900	1.20716000	-0.31323000
C	5.68205000	-0.41584000	-0.35456000
H	1.66114700	0.74512600	0.66411700
H	3.30527800	-1.12774700	0.92477000
H	3.25215800	-1.42667200	-0.80421600
H	-1.57960500	-2.47113300	0.45983500
H	-3.91761600	-1.74664900	0.43435100
H	-0.31748000	1.51913900	-0.50535200
H	-2.65779600	2.24752600	-0.53013600
H	0.78611000	-1.78687000	-0.81562500
H	1.68424000	0.53174900	-1.08052800

C	4.42714100	1.42447000	0.83212400
H	6.51946100	0.26437300	-0.54354100
H	5.89338000	-0.94892400	0.58056700
H	5.66274500	-1.15632400	-1.16157100
H	4.19047100	0.85611500	-1.22453700
H	5.27400600	2.09770800	0.66116600
H	3.52237800	2.03844200	0.87122600
H	4.56271400	0.96663800	1.81993300
C	-4.86339100	0.80993500	-0.08177900
H	-4.95805000	1.87145200	-0.30962300
C	-5.98542400	0.11308100	0.13639700
H	-5.98430900	-0.94757700	0.36938700
H	-6.95720700	0.59284000	0.08735600
H	0.82003400	-1.62241300	0.92181600

[Zr]-H

C	-1.42237500	-2.23674200	-0.47980900
C	-1.53645100	-1.49432700	-1.72213200
C	-2.15613100	-1.44908200	0.50727400
C	-2.17065600	-0.25609200	-1.48025200
C	-2.56626100	-0.19541500	-0.10293200
Zr	-0.06287000	-0.26734200	-0.03848700
C	1.24523900	-2.25079400	0.42731500
C	2.04452000	-1.49209400	-0.53841100
C	1.33000000	-1.50507300	1.66596100
C	2.51369800	-0.27346000	0.08903200
C	2.00480600	-0.28106500	1.43631000
Si	-0.09223200	-3.54238700	-0.03392100
C	0.37416900	-4.66801100	-1.46775200
C	-0.56833900	-4.68189500	1.38684100
C	3.32702000	0.66724400	-0.61627600
C	2.36811400	-1.72600200	-1.90069300
C	3.63855200	0.35986600	-1.93655800
C	3.16633600	-0.81040800	-2.56576300
C	-1.09912500	-1.92035100	-3.09818500
C	0.86519000	-1.91989500	3.03934700
C	3.83046800	1.90581400	0.02578800
C	-3.21700400	0.83054200	0.66550000
C	-2.48163800	-1.69034300	1.87250900
C	-3.47304800	0.53898200	2.00091900
C	-3.13518200	-0.70770200	2.58728700
C	-3.64997800	2.11571200	0.06133600
C	4.45072600	1.87648600	1.28760900

C	4.93877100	3.04819700	1.86492900
C	4.80933900	4.26773700	1.19668900
C	3.71713600	3.13760800	-0.64229700
C	4.19868400	4.30877400	-0.05846100
C	-2.79975900	2.86537300	-0.77158000
C	-3.21872000	4.08257100	-1.30704100
C	-4.49759800	4.56869600	-1.02787700
C	-4.93316700	2.61926800	0.33645100
C	-5.35286000	3.83300800	-0.20569600
H	-2.37304500	0.49164500	-2.23341600
H	2.22156300	0.45812800	2.19710300
H	-0.43238600	-5.39541100	-1.61461600
H	0.54507100	-4.17656800	-2.42583000
H	1.27776000	-5.23159700	-1.20974500
H	-1.47090700	-5.24177600	1.11722600
H	0.23637900	-5.41203500	1.53031600
H	-0.74415500	-4.20193000	2.34992800
H	2.06758300	-2.64371200	-2.39066800
H	4.28388600	1.03266400	-2.49206300
H	3.45859100	-1.00741500	-3.59261900
H	-2.26860000	-2.65018700	2.32622100
H	-3.96532000	1.28800700	2.61308900
H	-3.40834200	-0.88857300	3.62225300
H	4.58968000	0.92815000	1.79848300
H	5.43095600	3.00682900	2.83191900
H	5.18812200	5.17922500	1.64861100
H	3.23552300	3.17516300	-1.61522900
H	4.09722300	5.25326300	-0.58430700
H	-1.79454500	2.51232600	-0.99075700
H	-2.54453800	4.65294100	-1.93882200
H	-4.82485500	5.51411300	-1.44905300
H	-5.61267600	2.04305200	0.95720700
H	-6.35128400	4.20065100	0.00995100
H	-1.30651300	-1.12844600	-3.82124000
H	-0.03517100	-2.15115500	-3.16060200
H	-1.65298800	-2.81451800	-3.40292300
H	1.02537600	-1.11062400	3.75652600
H	-0.18669400	-2.20112400	3.08421800
H	1.45126600	-2.78202800	3.37533300
H	0.40220000	0.78527700	-1.45841000

[Zr]-BVPE-PP₁

C	1.57389800	-0.10673800	-1.61620600
---	------------	-------------	-------------

C	1.12716700	0.96387600	2.82994400
C	-0.21700300	1.04771200	2.31936500
C	1.92526900	1.83729900	1.97280000
C	-0.23732000	1.88228400	1.17460900
C	1.06010800	2.46176000	0.98782700
Zr	1.23157300	-0.28778300	0.72956000
C	2.31720800	-1.55122100	2.57941400
C	1.42227000	-2.49480600	1.92860500
C	3.42367200	-1.37585000	1.66450000
C	1.97820300	-2.85485600	0.63552000
C	3.17214700	-2.08788700	0.47024400
Si	1.85051900	-0.35868500	3.98754300
C	0.60133900	-1.07005400	5.20802000
C	3.27798800	0.23368000	5.06785700
C	1.36003800	-3.84860300	-0.19337400
C	0.17173600	-3.06000800	2.31435700
C	0.16352800	-4.39100900	0.26204800
C	-0.42692800	-3.99160200	1.48569000
C	-1.46651000	0.41084600	2.87967100
C	4.75898500	-0.72464700	1.92217600
C	1.96605100	-4.29510000	-1.47256700
C	1.53072400	3.57723900	0.20720300
C	3.30016500	2.20432800	2.02313300
C	2.88758600	3.86217800	0.29177200
C	3.76363600	3.17419600	1.16335000
C	0.63394200	4.52199000	-0.51141200
C	3.33301900	-4.61555500	-1.55811900
C	3.88325000	-5.06596900	-2.75717000
C	3.08207000	-5.19708100	-3.89363800
C	1.16807200	-4.44393500	-2.62108600
C	1.72286200	-4.88603100	-3.82144900
C	-0.50933000	4.11757500	-1.21836800
C	-1.32039800	5.04557100	-1.87137400
C	-1.01466000	6.40566100	-1.82511000
C	0.91927400	5.90153500	-0.46242300
C	0.10911800	6.82899400	-1.11308000
C	2.33316700	0.91757700	-2.45050900
C	3.85841000	0.79032600	-2.30923600
C	4.67878200	1.58298400	-3.34645100
C	0.11325300	-0.13021900	-1.64405700
C	-0.58530500	-1.09880300	-0.85690700
C	-1.99320700	-1.04725300	-0.69217700
C	-2.75791000	-0.07497700	-1.31896100
C	-0.69343500	0.84969800	-2.28386400

C	-2.06847500	0.84923900	-2.14575700
C	6.17368200	1.26050100	-3.20598700
H	-1.13414000	2.12874900	0.62486400
H	3.84987100	-2.14253400	-0.36980500
H	0.39443700	-0.31731100	5.97716100
H	-0.35758500	-1.37854800	4.79212000
H	1.04422600	-1.93550500	5.71379700
H	2.86381500	0.86545100	5.86198200
H	3.74994300	-0.62938300	5.55106100
H	4.06208500	0.81032000	4.57710500
H	-0.26570000	-2.83041100	3.27790600
H	-0.31514200	-5.17072800	-0.32179000
H	-1.35263600	-4.46541800	1.79838700
H	3.96023900	1.77667700	2.76288400
H	3.28842000	4.67471000	-0.30406100
H	4.80779400	3.47007200	1.19833100
H	3.95751100	-4.54992000	-0.67259100
H	4.93679000	-5.32507600	-2.80110000
H	3.51304200	-5.54502400	-4.82730700
H	0.11125500	-4.19681500	-2.57547500
H	1.09312300	-4.98680900	-4.70016200
H	-0.75458200	3.06771200	-1.28415900
H	-2.19359000	4.70379100	-2.42006900
H	-1.64841700	7.12833500	-2.32967000
H	1.76517900	6.25427900	0.11847200
H	0.34985400	7.88601100	-1.05218000
H	-2.32605800	0.65298500	2.25062000
H	-1.40973600	-0.67858000	2.95465400
H	-1.66484200	0.79526500	3.88556300
H	5.03843400	-0.01841600	1.13585000
H	4.80189000	-0.21593300	2.88210700
H	5.52360000	-1.50962100	1.94148600
H	2.02076500	1.93367100	-2.18706200
H	4.15918800	1.10256400	-1.29800300
H	4.13119100	-0.27079700	-2.40026300
H	-0.10663100	-2.05061300	-0.62733700
H	-2.46782800	-1.82641800	-0.10507600
H	-0.22108200	1.57726600	-2.93411200
H	-2.65062500	1.58610600	-2.69539000
H	1.98640000	-1.11099700	-1.75296300
H	2.07285300	0.78114200	-3.51286800
C	4.44180100	3.09817600	-3.26106400
H	6.76382900	1.77803200	-3.96890000
H	6.55346000	1.57621300	-2.22601600

H	6.36447900	0.18652700	-3.30855500
H	4.35566700	1.24724800	-4.34347900
H	5.03534300	3.62732000	-4.01351300
H	3.39300500	3.36501100	-3.42463200
H	4.73720100	3.48334700	-2.27716400
C	-4.26737200	0.02125000	-1.20991800
H	-4.52921400	1.00463700	-0.79562300
C	-4.96739000	-1.06801100	-0.37654700
H	-4.56538300	-1.06197100	0.64488900
H	-4.69169900	0.01730700	-2.22255700
H	-4.73984500	-2.05341900	-0.80145300
C	-6.46743900	-0.86911700	-0.32994700
C	-7.05702600	-0.05716500	0.65078600
C	-7.30400100	-1.45860200	-1.28425500
C	-8.42961700	0.16279800	0.67577500
H	-6.43105200	0.40332800	1.41249400
C	-8.67989700	-1.23994500	-1.26105300
H	-6.87739500	-2.10113100	-2.05127200
C	-9.27456100	-0.42245600	-0.28522800
H	-8.85027400	0.78877800	1.45651400
H	-9.30925700	-1.71267700	-2.01067000
C	-10.73296100	-0.22408900	-0.30895100
H	-11.25398300	-0.79132500	-1.07935000
C	-11.45875800	0.56462200	0.49280400
H	-12.53564300	0.63145300	0.38037800
H	-11.02023500	1.17016200	1.28063900

[TS1]

C	1.55688400	-0.31433200	-1.56551100
C	0.82753600	1.20938700	2.88800100
C	-0.36508500	1.36805600	2.09978300
C	1.84595100	2.01813000	2.22859100
C	-0.06569200	2.13870500	0.94076700
C	1.28277000	2.62083400	1.03577700
Zr	1.18025800	-0.14278800	0.81792900
C	1.82319800	-1.40621300	2.84304100
C	0.98328400	-2.34178200	2.11358300
C	3.06755200	-1.34549600	2.10369600
C	1.69952400	-2.80403800	0.93983800
C	2.95216400	-2.11400700	0.92192300
Si	1.23980900	-0.15455200	4.15063600
C	-0.24650400	-0.71565400	5.16543400

C	2.57258600	0.28742500	5.40725900
C	1.14873300	-3.80731200	0.07993600
C	-0.32824000	-2.83782600	2.36153600
C	-0.12319600	-4.27479100	0.39535700
C	-0.85103800	-3.79323800	1.51084100
C	-1.76009800	0.90100500	2.44232300
C	4.38860800	-0.76000400	2.53471400
C	1.89329600	-4.35159900	-1.08349600
C	1.99277500	3.67106100	0.34886100
C	3.13188000	2.42436300	2.68531500
C	3.25791900	3.98527100	0.82329000
C	3.82113000	3.37684800	1.97249700
C	1.37709200	4.52569800	-0.69794600
C	3.23708700	-4.75005500	-0.96800400
C	3.91348600	-5.29225900	-2.05987400
C	3.26403400	-5.43975700	-3.28752300
C	1.24723700	-4.51750100	-2.32163000
C	1.92870600	-5.05195500	-3.41443100
C	0.58146400	3.99915000	-1.72503400
C	0.02663300	4.82510300	-2.70192400
C	0.24932200	6.20222100	-2.66627700
C	1.58463500	5.91804000	-0.66872600
C	1.02877000	6.74499300	-1.64264100
C	2.44357500	0.46965000	-2.53555500
C	3.75626000	-0.26409900	-2.85584100
C	4.63560600	0.40381800	-3.93214000
C	0.11176500	-0.17025600	-1.59762000
C	-0.67794300	-0.96701500	-0.70624300
C	-2.07842600	-0.76203700	-0.57398500
C	-2.74235600	0.20640200	-1.30632200
C	-0.59820900	0.80822800	-2.35159100
C	-1.96243700	0.96540200	-2.22149000
C	5.80900900	-0.51516000	-4.30382700
H	4.27011100	1.39904900	0.25681900
H	4.23309500	0.82396800	-0.21266100
H	-0.79459400	2.43679400	0.20023000
H	3.74502600	-2.25804300	0.20153500
H	-0.44736400	0.04380300	5.92989100
H	-1.17317900	-0.86761800	4.61135500
H	-0.00548000	-1.64679800	5.69022200
H	2.31243000	1.21540400	5.92825000
H	2.60723800	-0.50935400	6.15916300
H	3.58005600	0.39234300	5.00320500
H	-0.87705200	-2.53149100	3.24341500

H	-0.55675200	-5.06283100	-0.21208200
H	-1.82872400	-4.21733100	1.71921900
H	3.52475500	2.05874200	3.62489900
H	3.82096700	4.76723700	0.32471600
H	4.79277800	3.71421100	2.32062700
H	3.74143800	-4.67273500	-0.00970900
H	4.94589100	-5.60968600	-1.94856500
H	3.79313600	-5.86010400	-4.13717000
H	0.21052100	-4.21192700	-2.43105400
H	1.41593700	-5.16548700	-4.36474900
H	0.41612600	2.93228100	-1.76925300
H	-0.57655700	4.39307500	-3.49578000
H	-0.18429200	6.84710100	-3.42436600
H	2.16148400	6.35764900	0.13881500
H	1.19678400	7.81667300	-1.59585800
H	-2.44991500	1.14286600	1.63230300
H	-1.83682800	-0.17245000	2.63337300
H	-2.10373500	1.41615300	3.34580200
H	5.12524900	-0.86300400	1.73477400
H	4.34683600	0.29254000	2.80823300
H	4.75955700	-1.31779800	3.40169600
H	2.65406000	1.47643300	-2.15710700
H	4.35238900	-0.38908600	-1.93949800
H	3.50628000	-1.27949500	-3.19273400
H	-0.30733400	-1.94518500	-0.40670300
H	-2.62677300	-1.42771400	0.08376800
H	-0.06419500	1.39024600	-3.09369200
H	-2.46908100	1.68934500	-2.85620800
H	1.84468600	-1.36850000	-1.52331900
H	1.90980900	0.61389400	-3.48684700
C	5.14869800	1.78847200	-3.50748300
H	6.41753600	-0.07602800	-5.10069700
H	6.46567200	-0.68096000	-3.44072900
H	5.45890600	-1.49363100	-4.64995700
H	4.01403700	0.53399400	-4.83100700
H	5.77049900	2.22918500	-4.29335000
H	4.33425900	2.49096600	-3.30429000
H	5.76480100	1.71527800	-2.60259700
C	-4.23516000	0.46353900	-1.22680600
H	-4.38569100	1.46401000	-0.79932400
C	-5.05312400	-0.56752600	-0.43594100
H	-4.83915500	-1.56769200	-0.83213800
H	-4.63291000	0.52500100	-2.24779000
H	-4.71403700	-0.57820600	0.61108000

C	-6.55529900	-0.34804900	-0.47140000
C	-7.13502400	0.92473000	-0.40494600
C	-7.41769100	-1.45354900	-0.53966200
C	-8.51986000	1.08216600	-0.40898500
H	-6.51025900	1.81154100	-0.34486700
C	-8.79891600	-1.29911600	-0.54097100
H	-6.99639800	-2.45479100	-0.59579000
C	-9.38500500	-0.02191800	-0.47815800
H	-8.94209700	2.08259700	-0.35870000
H	-9.42824700	-2.18183300	-0.59563000
C	-10.83926700	0.20459800	-0.48385100
H	-11.13467400	1.25008800	-0.40265500
C	-11.80464600	-0.71778500	-0.57874400
H	-11.59970600	-1.78070000	-0.66716800
H	-12.85071300	-0.43054700	-0.57213600

[IM1]

C	1.60423200	-0.24444700	-1.67308700
C	0.64475200	1.05645500	2.93738600
C	-0.53805300	1.10253900	2.11799500
C	1.57791000	1.99747900	2.34249100
C	-0.31288600	1.98209000	1.02018200
C	0.96829200	2.59828700	1.16611600
Zr	1.29593500	-0.07982900	0.80349700
C	1.88495100	-1.43813400	2.79838500
C	1.13127700	-2.40124300	2.00898500
C	3.14107400	-1.26287700	2.10492400
C	1.91767000	-2.77839300	0.85194000
C	3.11287700	-2.00131400	0.89343500
Si	1.16581100	-0.31293700	4.14955700
C	-0.27244600	-1.04987100	5.11973800
C	2.42381500	0.20423100	5.45547400
C	1.47310200	-3.79635300	-0.05283900
C	-0.13073100	-3.02974300	2.22077000
C	0.24486200	-4.38176800	0.21990800
C	-0.54651900	-4.00153400	1.33605800
C	-1.87517100	0.46481100	2.40708200
C	4.40612600	-0.59882700	2.58966700
C	2.28487000	-4.22708200	-1.22061900
C	1.60156400	3.72243200	0.51550500
C	2.83454900	2.48651900	2.81426100
C	2.84527100	4.10243200	0.99502500
C	3.45471900	3.49992600	2.12652400

C	0.92685500	4.56435300	-0.50533200
C	3.65368300	-4.52293500	-1.09241600
C	4.39399300	-4.95333000	-2.19295400
C	3.78373600	-5.09129700	-3.44165200
C	1.68021700	-4.38211100	-2.48067300
C	2.42412600	-4.80634800	-3.58142400
C	0.14609800	4.02086300	-1.53611800
C	-0.46123600	4.83933200	-2.48796400
C	-0.30908400	6.22485500	-2.42375900
C	1.06058300	5.96502900	-0.44641300
C	0.45231400	6.78386300	-1.39535500
C	2.36740700	0.61489500	-2.67811800
C	3.87059700	0.30189800	-2.74302900
C	4.64010900	1.04616900	-3.85337700
C	0.15815600	-0.19787300	-1.63588000
C	-0.55560800	-1.07131400	-0.75956300
C	-1.96882200	-0.99562500	-0.63791000
C	-2.71052600	-0.07751000	-1.35868500
C	-0.62645500	0.74445300	-2.36765300
C	-1.99740000	0.77841000	-2.24453400
C	6.07626700	0.51162400	-3.95489300
H	3.10621800	0.93734500	0.49361300
H	2.90812500	0.72320300	-0.23372500
H	-1.05386000	2.22459300	0.27166500
H	3.93465400	-2.06392900	0.19327500
H	-0.54579200	-0.34303700	5.91173500
H	-1.17678800	-1.25974800	4.54851900
H	0.04583400	-1.97658000	5.61008300
H	2.05140000	1.06981800	6.01456400
H	2.52964900	-0.62158800	6.16841400
H	3.42295200	0.44081600	5.08817000
H	-0.72449000	-2.80036700	3.09688100
H	-0.10712900	-5.18479700	-0.42013700
H	-1.48433500	-4.52013000	1.51103400
H	3.25557400	2.11734900	3.74010400
H	3.35389900	4.93414800	0.51898200
H	4.40353300	3.89191000	2.48007700
H	4.13082900	-4.45341400	-0.11961300
H	5.44626100	-5.19275300	-2.07206400
H	4.36223300	-5.42537400	-4.29743000
H	0.62439500	-4.15518200	-2.59873800
H	1.94098300	-4.91432100	-4.54785400
H	0.02909000	2.94857600	-1.60519900
H	-1.05219600	4.39433700	-3.28379200

H	-0.78449500	6.86319900	-3.16203800
H	1.62092900	6.41657700	0.36605600
H	0.56443900	7.86150800	-1.32450700
H	-2.58395300	0.69530500	1.61058800
H	-1.82996000	-0.62244600	2.50381400
H	-2.27869100	0.86421800	3.34342400
H	5.12501700	-0.50755300	1.77049300
H	4.25789000	0.39294000	3.01187400
H	4.86776500	-1.22406400	3.36237300
H	2.21146400	1.68060300	-2.47228300
H	4.35271500	0.53010000	-1.77962800
H	3.99250800	-0.77904000	-2.89587100
H	-0.09298900	-2.00279800	-0.45111900
H	-2.46155000	-1.71995200	0.00118800
H	-0.13902800	1.39022800	-3.08872600
H	-2.56436900	1.47044600	-2.86354500
H	1.99186600	-1.26427800	-1.62100300
H	1.94701100	0.43835500	-3.68086500
C	4.64326000	2.56904100	-3.64932900
H	6.62248400	0.99968800	-4.76817100
H	6.63141200	0.69803800	-3.02701700
H	6.09126200	-0.56742700	-4.14250400
H	4.13354100	0.83190400	-4.80637600
H	5.20841300	3.06583000	-4.44424600
H	3.63485700	2.99448600	-3.65282200
H	5.11727400	2.83324300	-2.69518100
C	-4.22187600	0.02964600	-1.29894000
H	-4.49265300	1.01404300	-0.89130300
C	-4.95639100	-1.05929300	-0.49449900
H	-4.69138400	-2.04517600	-0.89580900
H	-4.61127400	0.03126600	-2.32529900
H	-4.61590900	-1.03910000	0.54863900
C	-6.45906000	-0.88027300	-0.53621600
C	-7.23131400	-1.49396900	-1.52874600
C	-7.11516800	-0.06547400	0.39887400
C	-8.60939500	-1.29672100	-1.58606400
H	-6.75223400	-2.13915400	-2.26182500
C	-8.49008300	0.13346400	0.34336900
H	-6.53993200	0.41405900	1.18831800
C	-9.27053300	-0.47756000	-0.65545900
H	-9.18832600	-1.78830200	-2.36369100
H	-8.96346300	0.76391700	1.08953400
C	-10.72832900	-0.30422100	-0.76315700
H	-11.19351200	-0.87658100	-1.56488100

C	-11.51391000	0.46602400	-0.00075100
H	-11.13338900	1.07278100	0.81572900
H	-12.58341700	0.51446800	-0.17567700

[TS2]

C	1.62289700	-0.26789800	-1.70680600
C	0.63814000	1.09433500	2.96544700
C	-0.53753500	1.13160900	2.13335900
C	1.57282900	2.04069600	2.37829400
C	-0.30009300	2.00244700	1.03093000
C	0.97673800	2.62792600	1.19175300
Zr	1.28710900	-0.05477700	0.85230100
C	1.88058600	-1.39687500	2.84280700
C	1.12911000	-2.37075600	2.06189100
C	3.13901200	-1.22621500	2.14959800
C	1.91591000	-2.75426700	0.90850400
C	3.11136200	-1.97558500	0.94744100
Si	1.15712300	-0.26647900	4.18763000
C	-0.28425000	-0.99852100	5.15700900
C	2.41567100	0.25397700	5.49111100
C	1.47528600	-3.78291300	0.01298500
C	-0.12875400	-3.00393200	2.28113900
C	0.25055700	-4.37229000	0.29227500
C	-0.54116900	-3.98587200	1.40577200
C	-1.87588500	0.49088000	2.40980800
C	4.39539100	-0.53893000	2.62103300
C	2.28740800	-4.22002800	-1.15244800
C	1.61425900	3.74608900	0.53847400
C	2.81636200	2.54010400	2.86564100
C	2.84304700	4.14624900	1.04013400
C	3.43717100	3.55865200	2.18552300
C	0.95675900	4.56194300	-0.51423500
C	3.65925700	-4.50271000	-1.02600800
C	4.39932300	-4.94005100	-2.12403200
C	3.78594000	-5.09897100	-3.36870100
C	1.68003800	-4.39545400	-2.40875800
C	2.42342500	-4.82740400	-3.50694300
C	0.22548500	3.98774400	-1.56421900
C	-0.36592400	4.77923900	-2.54836500
C	-0.24584700	6.16858200	-2.49847600
C	1.05967700	5.96541000	-0.47135300
C	0.46761000	6.75777900	-1.45271300
C	2.34877000	0.52172000	-2.80016400

C	3.85815600	0.23948200	-2.85295300
C	4.60163900	0.92316400	-4.01855800
C	0.15849400	-0.20802200	-1.64424800
C	-0.55293700	-1.07924700	-0.77310200
C	-1.96265900	-1.01257500	-0.65841900
C	-2.70612200	-0.10014700	-1.39067700
C	-0.61937500	0.71992100	-2.39005800
C	-1.99424100	0.75200200	-2.27441500
C	6.04561700	0.40651000	-4.10259100
H	2.89810500	0.78500100	0.20475700
H	2.50946100	0.46848000	-0.57851300
H	-1.03320800	2.24125200	0.27294400
H	3.93215600	-2.03676800	0.24591000
H	-0.55485400	-0.28962900	5.94815000
H	-1.18911500	-1.20354000	4.58469500
H	0.02863200	-1.92649100	5.64838400
H	2.04955100	1.12614600	6.04401200
H	2.51631800	-0.56742200	6.20993100
H	3.41578400	0.48042500	5.11995400
H	-0.72256300	-2.76990300	3.15602900
H	-0.09761400	-5.18352500	-0.33946700
H	-1.47573100	-4.50804700	1.58748500
H	3.22771200	2.17702900	3.79828200
H	3.35217700	4.97836400	0.56495100
H	4.37613900	3.96125500	2.55304900
H	4.13924000	-4.41804600	-0.05588400
H	5.45400400	-5.16901400	-2.00397300
H	4.36416400	-5.43915600	-4.22224900
H	0.62155500	-4.18036000	-2.52553300
H	1.93755100	-4.95227200	-4.46998900
H	0.13530500	2.91191100	-1.62042500
H	-0.91864000	4.31097100	-3.35832200
H	-0.70845000	6.78642400	-3.26190000
H	1.58372700	6.43914600	0.35271000
H	0.55510600	7.83846200	-1.39425400
H	-2.57277600	0.70619100	1.59827000
H	-1.82677700	-0.59466600	2.52366900
H	-2.29822100	0.90164700	3.33292100
H	5.11882000	-0.47398500	1.80393100
H	4.23597000	0.46906700	2.99825700
H	4.85288200	-1.12964500	3.42294800
H	2.16991200	1.59597000	-2.67434800
H	4.33262100	0.54866400	-1.90924700
H	4.00552900	-0.84624200	-2.93138500

H	-0.07084600	-1.98204600	-0.41282700
H	-2.45458100	-1.73163600	-0.01304200
H	-0.13123400	1.36741600	-3.10867400
H	-2.55848200	1.44237300	-2.89744500
H	1.98811300	-1.29568700	-1.64604400
H	1.90906400	0.24804000	-3.77106200
C	4.58133900	2.45575900	-3.91163100
H	6.57494100	0.85227400	-4.95054800
H	6.60684500	0.65877900	-3.19431200
H	6.07691800	-0.68169700	-4.22367900
H	4.08863500	0.63947300	-4.94983400
H	5.12567600	2.90973600	-4.74567000
H	3.56589900	2.86410100	-3.92601000
H	5.06451000	2.78735900	-2.98382600
C	-4.21795700	0.00299000	-1.33321300
H	-4.48977100	0.99339700	-0.94174000
C	-4.95111300	-1.07348600	-0.51103600
H	-4.60790000	-1.03839300	0.53081400
H	-4.60650900	-0.01265000	-2.35968300
H	-4.68938600	-2.06576600	-0.89850500
C	-6.45351800	-0.89115100	-0.55177400
C	-7.23047500	-1.52025900	-1.53084600
C	-7.10405900	-0.05697900	0.37001900
C	-8.60795100	-1.31864400	-1.58852200
H	-6.75574600	-2.18082300	-2.25297200
C	-8.47827400	0.14635500	0.31401200
H	-6.52518900	0.43426900	1.14954200
C	-9.26340700	-0.47927100	-0.67205200
H	-9.19068800	-1.82205600	-2.35564100
H	-8.94759700	0.79145000	1.05012600
C	-10.72054600	-0.30039700	-0.78014000
H	-11.19213200	-0.89309100	-1.56310000
C	-11.49805000	0.49793000	-0.03862300
H	-11.10994600	1.12704800	0.75707200
H	-12.56789800	0.54832600	-0.21084100

[IM2]

C	2.77443000	-1.45989500	2.20978400
C	0.11280800	2.01066300	-2.83250100
C	-0.58848100	0.76244300	-2.66517100
C	1.52850400	1.66834400	-2.85744300
C	0.35475400	-0.28475700	-2.48569700
C	1.67836800	0.24066500	-2.66502900

Zr	0.53829600	1.35414200	-0.50009200
C	-0.29601200	3.66992900	-0.62870300
C	-1.22570500	3.05970500	0.31061000
C	0.95540600	3.79833700	0.09011100
C	-0.53094500	2.79317200	1.55408500
C	0.82808300	3.19669500	1.36202200
Si	-0.55313800	3.76396300	-2.51052100
C	-2.34319600	3.99451300	-3.05407600
C	0.41070900	5.15547200	-3.33872200
C	-1.23042800	2.30308400	2.70869700
C	-2.61861900	2.76833500	0.22307500
C	-2.58739200	2.05686600	2.56081500
C	-3.26927000	2.27826400	1.33561000
C	-2.07644000	0.52011000	-2.73991900
C	2.20468500	4.53431100	-0.31687000
C	-0.55564000	2.10344100	4.01687300
C	2.96014400	-0.38799100	-2.82536400
C	2.67677600	2.46312000	-3.12171000
C	4.04045900	0.44904600	-3.07168000
C	3.90661900	1.84924600	-3.20995000
C	3.14003800	-1.86051300	-2.88084900
C	0.30547100	3.07897400	4.55151900
C	0.90329300	2.89492500	5.79766000
C	0.65731500	1.73274900	6.53170000
C	-0.80323300	0.94310600	4.77257200
C	-0.20001400	0.75870300	6.01619200
C	2.50058400	-2.73118600	-1.98492100
C	2.69779900	-4.11022800	-2.06168500
C	3.53322100	-4.64961600	-3.04103100
C	3.97539200	-2.41916800	-3.86630100
C	4.17056700	-3.79664700	-3.94411900
C	3.75911600	-2.61465300	1.98562300
C	5.14328600	-2.31407100	2.57772600
C	6.16539200	-3.46285500	2.46401500
C	1.39571400	-1.61950200	1.59772800
C	0.51650900	-0.51963100	1.56094900
C	-0.78026400	-0.63028800	1.02403700
C	-1.25457400	-1.85636600	0.51610600
C	0.90394800	-2.83754800	1.10840700
C	-0.38515800	-2.95150800	0.58009400
C	7.44160000	-3.11805900	3.24612600
H	2.31352000	1.28551100	-0.11462600
H	3.21215700	-0.53149200	1.82045800
H	0.09859000	-1.33064300	-2.38377300

H	1. 61760100	3. 15446900	2. 09908900
H	-2. 35458500	4. 12818500	-4. 14198800
H	-3. 01825800	3. 17004500	-2. 82341100
H	-2. 75384200	4. 90872200	-2. 61134700
H	0. 46629500	4. 98330100	-4. 41934200
H	-0. 14256700	6. 08940600	-3. 18636200
H	1. 42301900	5. 31699600	-2. 96672500
H	-3. 17655800	3. 00118900	-0. 67518900
H	-3. 15742100	1. 72817600	3. 42422600
H	-4. 33938300	2. 09903200	1. 29356500
H	2. 57907700	3. 52040200	-3. 33099600
H	5. 02502900	0. 00811800	-3. 18857900
H	4. 78920400	2. 44096700	-3. 43273100
H	0. 47445400	4. 00364200	4. 00878000
H	1. 55255900	3. 66624400	6. 20083100
H	1. 12451900	1. 59076000	7. 50131300
H	-1. 46324500	0. 17711300	4. 37576200
H	-0. 40049900	-0. 14585200	6. 58253600
H	1. 87078600	-2. 32709600	-1. 20285100
H	2. 19924500	-4. 76600000	-1. 35327500
H	3. 68266600	-5. 72310500	-3. 10330100
H	4. 45297400	-1. 76965800	-4. 59325900
H	4. 81381300	-4. 20466200	-4. 71785800
H	-2. 29347600	-0. 54263300	-2. 61417900
H	-2. 65171400	1. 06730800	-1. 98855700
H	-2. 45323200	0. 82042200	-3. 72303200
H	3. 01976900	4. 30285700	0. 37287700
H	2. 54822200	4. 29368100	-1. 32093700
H	2. 02151600	5. 61425600	-0. 27374600
H	3. 84387200	-2. 81145700	0. 91037700
H	5. 55845200	-1. 41818700	2. 09237300
H	5. 02336900	-2. 05661500	3. 63930300
H	0. 81801800	0. 39562400	2. 06978600
H	-1. 48321600	0. 19639000	1. 12436500
H	1. 53558300	-3. 71863300	1. 13873600
H	-0. 72215200	-3. 91914000	0. 21667400
H	2. 64868600	-1. 29630000	3. 29005700
H	3. 36886700	-3. 53287400	2. 44542300
C	6. 50356500	-3. 80862700	1. 00533400
H	8. 16211500	-3. 94145900	3. 21001400
H	7. 93107500	-2. 23137500	2. 82518800
H	7. 22372100	-2. 91003800	4. 29925000
H	5. 71672400	-4. 35393600	2. 92900700
H	7. 24350700	-4. 61423600	0. 95911900

H	5.62695500	-4.13742400	0.43832900
H	6.92933100	-2.93962200	0.48815900
C	-2.67412700	-2.00902900	0.02277500
H	-3.09395700	-1.02677700	-0.21646900
H	-2.68758500	-2.59470000	-0.90420100
C	-3.60624300	-2.70492700	1.05315700
H	-3.20045400	-3.69584900	1.28737800
H	-3.59145600	-2.13030100	1.98688800
C	-5.02377500	-2.82914800	0.54141300
C	-5.97647300	-1.83340300	0.80573000
C	-5.41513800	-3.91969100	-0.24424400
C	-7.26973000	-1.91954600	0.30208100
H	-5.70242200	-0.98344100	1.42760400
C	-6.70979000	-4.00782600	-0.75077200
H	-4.70341100	-4.71450500	-0.45652200
C	-7.66653600	-3.01165600	-0.49143000
H	-7.98111900	-1.13306700	0.53389000
H	-6.99141400	-4.86779300	-1.35288900
C	-9.02126000	-3.15761800	-1.04847700
H	-9.16587300	-4.04832300	-1.65864700
C	-10.06105600	-2.33125400	-0.88203100
H	-10.00628500	-1.42539200	-0.28535900
H	-11.01940700	-2.54348100	-1.34379800

BVPE-PP₁

C	4.20930700	-0.84638600	0.99880100
C	4.99874900	-0.04405100	-0.05573800
C	6.50748700	-0.02333300	0.21930100
C	7.36357100	0.67560900	-0.85554800
C	-3.89762700	0.18809900	0.16509600
C	-4.73984700	1.16741300	0.72162900
C	-6.10237600	1.19026200	0.46227700
C	-6.69639000	0.22567000	-0.37428100
C	-4.48512500	-0.76979000	-0.66644800
C	-5.85584300	-0.74911000	-0.92920600
C	8.85829000	0.48338800	-0.55977200
H	4.60077500	0.97706900	-0.08731100
H	6.69396100	0.45773000	1.19136600
H	6.85960800	-1.05933600	0.32442500
H	-4.31038500	1.92634300	1.37207400
H	-6.71336400	1.96605600	0.91359200
H	-3.87894200	-1.54623000	-1.12096300
H	-6.28355300	-1.50789500	-1.58006600

H	4.58885200	-1.87598300	1.02161900
H	4.80943700	-0.47568900	-1.04805500
C	7.03030600	2.16854300	-0.99611700
H	9.47984000	0.93634900	-1.33970900
H	9.13120300	0.95143600	0.39406700
H	9.12104900	-0.57822000	-0.49572100
H	7.14720800	0.18976100	-1.81927500
H	7.66503200	2.64145000	-1.75327400
H	5.98956900	2.33329200	-1.29046400
H	7.19699700	2.69592400	-0.04844300
C	-8.13381200	0.19734500	-0.68494200
H	-8.43310500	-0.60586800	-1.35790500
C	-9.08313900	1.02943000	-0.23947300
H	-8.87388000	1.85466300	0.43460300
H	-10.11780600	0.90647000	-0.54152100
H	4.40731800	-0.42154300	1.99112700
C	-2.41487900	0.22583300	0.49379400
H	-2.01966800	1.20564400	0.19269400
H	-2.30347000	0.18892400	1.58594300
C	-1.55960700	-0.87517200	-0.13570300
H	-1.67216400	-0.83767400	-1.22763700
H	-1.95499600	-1.85435600	0.16670300
C	-0.07560500	-0.83379400	0.19356400
C	0.76711200	-1.81399100	-0.35335000
C	0.50828800	0.13067300	1.02162400
C	2.13247500	-1.82773600	-0.08599800
H	0.34169300	-2.58153400	-0.99656500
C	1.87945500	0.11594700	1.28946600
H	-0.10187600	0.90597000	1.47333500
C	2.71820700	-0.85908700	0.74213700
H	2.75553900	-2.60500000	-0.52278300
H	2.30115000	0.87768600	1.94146500

IM3_{1,2}

C	-5.82996300	1.19320400	0.13756200
C	3.88697400	-1.56702500	0.34545200
C	3.58344900	-1.63856400	-1.06495100
C	2.83166300	-2.31979200	1.01256400
C	2.33992500	-2.29797800	-1.24279800
C	1.87879000	-2.78158300	0.02686500
Zr	1.91819400	-0.11807300	0.04939000
C	3.73116700	1.10786300	1.17508800
C	3.45424900	1.94548400	0.01679800

C	2.59544700	1.27640600	2.05659400
C	2.16099500	2.57785000	0.18632300
C	1.62805800	2.09248900	1.42335600
Si	5.01714800	-0.29577800	1.20558300
C	6.60183600	0.05900900	0.24869800
C	5.56466100	-0.77044000	2.94520900
C	1.68850000	3.55854400	-0.75337200
C	4.22974400	2.25515300	-1.13885400
C	2.48984400	3.80679300	-1.85742500
C	3.73648600	3.15951100	-2.05323800
C	4.42956700	-1.18805600	-2.23127100
C	2.41870300	0.76819200	3.46415100
C	0.43646900	4.33193200	-0.54652700
C	0.77083200	-3.61126600	0.39973700
C	2.63951400	-2.66929600	2.37708000
C	0.64531200	-3.92082700	1.74669600
C	1.56082300	-3.45683000	2.71922600
C	-0.16925300	-4.18721100	-0.59534700
C	0.09155000	4.84662200	0.71666300
C	-1.06185800	5.61156400	0.88565400
C	-1.89681100	5.87952700	-0.20148400
C	-0.40888500	4.62029000	-1.63456800
C	-1.56404600	5.38327600	-1.46374700
C	0.28901700	-4.74486800	-1.80334700
C	-0.60095100	-5.33138300	-2.70363900
C	-1.96633000	-5.37611000	-2.41620000
C	-1.54710800	-4.24632500	-0.31623700
C	-2.43510800	-4.83565300	-1.21645000
C	-6.88219700	0.09111000	0.30249200
C	-8.22215400	0.64767500	0.80527600
C	-9.35814500	-0.38816300	0.92332900
C	-4.45867100	0.77382300	-0.34940200
C	-3.44804100	1.75258300	-0.46437400
C	-2.18129600	1.43449800	-0.91812500
C	-1.86210600	0.10369600	-1.27483700
C	-4.14170800	-0.54502900	-0.70561100
C	-2.86853600	-0.87628300	-1.15756500
C	-10.68647300	0.31338600	1.24379500
H	0.56032900	-0.54755800	1.18633400
H	1.89613000	-2.51552000	-2.20497400
H	0.68104600	2.36764800	1.86563000
H	7.30774800	-0.75641800	0.44425700
H	6.49180400	0.13735600	-0.83319800
H	7.06385300	0.98281500	0.61407600

H	6.08157300	-1.73634200	2.92618000
H	6.28683000	-0.02228900	3.29219200
H	4.77148500	-0.82293400	3.69184800
H	5.22595700	1.84869400	-1.26114500
H	2.18706500	4.57178500	-2.56529700
H	4.33654100	3.43193400	-2.91616000
H	3.36917400	-2.38718400	3.12550000
H	-0.15449600	-4.58429400	2.05972500
H	1.42686000	-3.76327500	3.75208900
H	0.75150500	4.68428700	1.56231300
H	-1.30058700	6.01182400	1.86646400
H	-2.79181100	6.47956200	-0.06839800
H	-0.16349700	4.23555400	-2.62063800
H	-2.20155700	5.59136600	-2.31785800
H	1.35276800	-4.76449600	-2.01786400
H	-0.22363100	-5.77007900	-3.62255900
H	-2.65724600	-5.83750500	-3.11498400
H	-1.92135600	-3.81815700	0.60905300
H	-3.49422100	-4.87602500	-0.97866600
H	3.90375000	-1.36901200	-3.17301700
H	4.69800800	-0.13082200	-2.20150500
H	5.36049900	-1.76418300	-2.25864500
H	1.40461100	0.97571000	3.81364700
H	2.58461200	-0.30427000	3.56455200
H	3.11980500	1.28074600	4.13244700
H	-6.50647500	-0.66857200	0.99852300
H	-8.07262800	1.12657300	1.78426500
H	-8.54710000	1.44636300	0.12408900
H	-3.67238200	2.78225300	-0.19889600
H	-1.43946300	2.22045600	-1.00166000
H	-4.89531900	-1.32082300	-0.63268900
H	-2.64527700	-1.90414800	-1.42818300
H	-6.21203500	1.95787200	-0.55446200
H	-7.04223000	-0.41552000	-0.65898900
C	-9.05770500	-1.47534800	1.96668000
H	-11.51131900	-0.40475200	1.29351900
H	-10.63539500	0.82621300	2.21195700
H	-10.93870300	1.06085000	0.48389600
H	-9.46460800	-0.87789900	-0.05661600
H	-9.88800800	-2.18535800	2.03817900
H	-8.15787000	-2.04997800	1.72417500
H	-8.91508000	-1.03294300	2.96040100
C	-0.56912000	-0.29045700	-1.78919800
H	-0.48090900	-1.35157500	-2.02334800

C	0.53232100	0.49974700	-2.02080800
H	-5.70153200	1.71814800	1.09487500
H	1.33480200	0.09576800	-2.64002400
H	0.47356300	1.58152700	-1.95965700

TS3_{1,2}

C	5.70044400	-0.32196900	1.53069500
C	-4.09022100	0.63037100	0.82186400
C	-4.19353000	0.75486100	-0.61465500
C	-3.15676100	1.67126000	1.23707100
C	-3.28646300	1.74814000	-1.07053400
C	-2.67897400	2.37815900	0.06545400
Zr	-1.91746400	-0.15497600	-0.02624600
C	-2.93441600	-1.87955700	1.41281800
C	-2.76270300	-2.55673600	0.13315900
C	-1.59879000	-1.70804000	1.94204100
C	-1.34743700	-2.73911800	-0.12367900
C	-0.65141800	-2.16300200	0.98794300
Si	-4.51114000	-0.90631800	1.87425800
C	-6.12649500	-1.73727900	1.36998800
C	-4.67213200	-0.57162100	3.72200300
C	-0.89495200	-3.43839100	-1.29704600
C	-3.70844300	-3.06406600	-0.80679400
C	-1.86440000	-3.87604700	-2.18326200
C	-3.25164900	-3.69511800	-1.94143400
C	-5.15592600	0.06415600	-1.54938500
C	-1.19152000	-1.19747100	3.30189200
C	0.53790000	-3.74627800	-1.53915500
C	-1.80564300	3.51011400	0.18723000
C	-2.69940600	2.07928300	2.52282400
C	-1.41552600	3.86694600	1.47076600
C	-1.84946000	3.16137100	2.61861500
C	-1.36275200	4.29916700	-0.99076300
C	1.34836900	-4.28345300	-0.52356000
C	2.67617100	-4.62471200	-0.77936000
C	3.22294200	-4.42822400	-2.04991400
C	1.09790000	-3.56280600	-2.81660500
C	2.42912800	-3.89550900	-3.06822400
C	-2.26531900	4.67788100	-2.00131300
C	-1.84012400	5.44245800	-3.08683800
C	-0.50533400	5.84054700	-3.18905300
C	-0.02526100	4.72245800	-1.09909300
C	0.40003600	5.48095100	-2.18939200

C	6.83056800	0.33402900	0.70617800
C	8.22130000	0.05780800	1.29231200
C	9.39984900	0.60048800	0.45876500
C	4.32877500	-0.04865200	0.96129100
C	3.76351700	-0.89538200	-0.00364700
C	2.51961000	-0.62511700	-0.56893300
C	1.79538600	0.51327300	-0.17987100
C	3.60134800	1.09150600	1.34408800
C	2.36177400	1.36924400	0.78341700
C	10.73435100	0.11188800	1.04172600
H	-0.43371800	0.72928700	0.66111300
H	-3.18849900	2.06404400	-2.10013000
H	0.42085000	-2.14410300	1.12799100
H	-6.95359600	-1.16186200	1.80163800
H	-6.31076000	-1.80913800	0.29752100
H	-6.17660500	-2.74621100	1.79427100
H	-5.42292000	0.20695200	3.89685400
H	-5.03463200	-1.48693800	4.20392600
H	-3.75395200	-0.28072900	4.23330500
H	-4.76949900	-3.01719700	-0.59824600
H	-1.55783700	-4.43760600	-3.06006400
H	-3.96343500	-4.11272000	-2.64700000
H	-3.07214000	1.59794200	3.41807300
H	-0.79307600	4.74650100	1.60294100
H	-1.53198300	3.50771700	3.59738300
H	0.92673300	-4.47027900	0.45915800
H	3.28075900	-5.05771600	0.01205100
H	4.25592100	-4.69773400	-2.24786500
H	0.48617100	-3.15073000	-3.61445100
H	2.84388900	-3.74242500	-4.05997400
H	-3.31350100	4.40994200	-1.91447400
H	-2.55573600	5.73819300	-3.84812200
H	-0.17584100	6.43360500	-4.03647700
H	0.68849200	4.44831400	-0.32694800
H	1.43834300	5.79142800	-2.25645200
H	-4.92964200	0.32372000	-2.58713600
H	-5.14557200	-1.02277000	-1.47121000
H	-6.17630300	0.40235100	-1.33882000
H	-0.10626900	-1.07930800	3.35141800
H	-1.63915100	-0.23684900	3.55965200
H	-1.48768100	-1.91851700	4.07186300
H	6.64482000	1.41318700	0.65062600
H	8.27846900	0.47670400	2.30798400
H	8.34509900	-1.02830700	1.40583900

H	4.30653500	-1.77990600	-0.32401000
H	2.12948800	-1.29385600	-1.32795100
H	4.01741800	1.76511900	2.08858000
H	1.81111200	2.25086000	1.10247700
H	5.87145400	-1.40435900	1.57535300
H	6.78255800	-0.03899200	-0.32583400
C	9.38823000	2.13293600	0.34839900
H	11.57964400	0.45208000	0.43467600
H	10.88183000	0.49569700	2.05853400
H	10.77504800	-0.98174000	1.08967300
H	9.30539600	0.18707600	-0.55704300
H	10.24494500	2.48746200	-0.23402000
H	8.48372000	2.50835300	-0.14055300
H	9.44994300	2.59620600	1.34102000
C	0.49778600	0.88240400	-0.78199700
H	0.29157700	1.94964300	-0.74555400
C	-0.23700800	0.14787900	-1.73707200
H	5.74980200	0.04733500	2.56227200
H	-0.76516400	0.72070100	-2.49736200
H	0.12209700	-0.82914600	-2.05005100

PR3_{1,2}

C	5.97045300	-1.00785500	0.00785000
C	-4.30812600	0.94582200	-0.07000800
C	-3.79299300	1.24554700	-1.39103200
C	-3.56257700	1.80950400	0.84045900
C	-2.70582000	2.14410500	-1.28282400
C	-2.56159200	2.53969300	0.08886200
Zr	-2.04663800	-0.01735800	-0.08527700
C	-3.64460300	-1.68469200	0.70045100
C	-2.91344400	-2.33855500	-0.38377700
C	-2.71135200	-1.61331400	1.80441900
C	-1.56473800	-2.62889000	0.06066900
C	-1.44552900	-2.09168300	1.38759800
Si	-5.22561100	-0.63379000	0.48694700
C	-6.43474100	-1.29717600	-0.79606000
C	-6.22342400	-0.44284400	2.07327100
C	-0.65406100	-3.37333400	-0.75120200
C	-3.27504000	-2.66743600	-1.71911200
C	-1.07833200	-3.68893800	-2.03848400
C	-2.35490900	-3.32424200	-2.51882100
C	-4.30335200	0.75186800	-2.72179400
C	-2.97580200	-1.21794300	3.23555700

C	0.65581500	-3.84629300	-0.24172100
C	-1.68206200	3.47750600	0.73265500
C	-3.67949200	2.04671000	2.24046300
C	-1.82882900	3.63475500	2.10198200
C	-2.81924200	2.93914800	2.84269100
C	-0.68519900	4.27337500	-0.02819800
C	0.76234700	-4.44047900	1.02923600
C	1.98288100	-4.93923600	1.48105800
C	3.11984900	-4.84926100	0.67546600
C	1.80592000	-3.77158500	-1.04602700
C	3.02697900	-4.26320000	-0.58821600
C	-1.03676800	4.93887300	-1.21635100
C	-0.09969000	5.71044900	-1.90284700
C	1.20553300	5.82676800	-1.42000900
C	0.62895700	4.40988900	0.45390300
C	1.56619600	5.17616400	-0.23838100
C	6.91124900	0.21490600	0.06028700
C	8.38200900	-0.17984000	0.24664400
C	9.38285500	0.99344600	0.22129200
C	4.51832200	-0.62769800	-0.17693400
C	3.68039900	-0.40904400	0.92352600
C	2.35390600	-0.01190300	0.75170900
C	1.82172900	0.17378000	-0.52831800
C	3.97714400	-0.44170700	-1.45776400
C	2.65188200	-0.05045100	-1.63519500
C	10.82522700	0.46530100	0.22461200
H	-2.14310100	2.53480900	-2.11834600
H	-0.57735700	-2.17793400	2.02761500
H	-7.33258400	-0.66864600	-0.78058200
H	-6.07643700	-1.32214000	-1.82549400
H	-6.74318700	-2.31156500	-0.51952200
H	-6.96019500	0.35887700	1.95078700
H	-6.77883300	-1.37222100	2.24388300
H	-5.64888400	-0.23986100	2.97735400
H	-4.27958800	-2.49019200	-2.08259300
H	-0.42686500	-4.27751600	-2.67637200
H	-2.63880800	-3.61699800	-3.52514000
H	-4.47779900	1.58869200	2.81051700
H	-1.20611900	4.36049500	2.61545100
H	-2.92367500	3.15195400	3.90220900
H	-0.12324200	-4.55278200	1.64729600
H	2.04262600	-5.41095100	2.45732600
H	4.07015300	-5.23815200	1.02822300
H	1.74840800	-3.30343000	-2.02379900

H	3.90669300	-4.18657700	-1.21957100
H	-2.05804400	4.88630400	-1.58112100
H	-0.39304000	6.23069500	-2.80968600
H	1.93428000	6.42591500	-1.95704500
H	0.91885300	3.90254600	1.36987300
H	2.57797400	5.26394200	0.14555100
H	-3.67006600	1.12263100	-3.53128200
H	-4.33870700	-0.33560600	-2.80277500
H	-5.31869500	1.12671100	-2.88942500
H	-2.03939000	-1.18373700	3.79879500
H	-3.46440100	-0.25146700	3.34657200
H	-3.61752800	-1.97077500	3.70660400
H	6.58493000	0.87436900	0.87343900
H	8.49576300	-0.72551400	1.19529500
H	8.65742200	-0.89038700	-0.54529100
H	4.06895900	-0.55314100	1.92846400
H	1.72932900	0.15562900	1.62774100
H	4.60458400	-0.60633400	-2.33043900
H	2.26055200	0.08854100	-2.63943200
H	6.28559600	-1.66548300	-0.81201900
H	6.79819400	0.79307500	-0.86693000
C	9.16661700	1.97715900	1.38172100
H	11.54793700	1.28595000	0.16827000
H	11.03433000	-0.09717000	1.14275700
H	11.00998100	-0.20247300	-0.62382700
H	9.22741600	1.54134100	-0.72055900
H	9.90025300	2.78923400	1.34558300
H	8.17196600	2.43360700	1.35979200
H	9.28186800	1.47094100	2.34826900
C	0.40692600	0.68088600	-0.74393700
H	0.41975500	1.75031400	-0.97859500
C	-0.49776300	-0.07322100	-1.71108900
H	6.08450300	-1.58603400	0.93299100
H	-0.71542500	0.48437900	-2.62145300
H	-0.13351100	-1.07302000	-1.94930300
H	-0.03503400	0.68753900	0.32409300

IM3_{2,1}

C	0.77684200	-0.59531400	-2.30149400
C	1.08864300	1.40122900	2.31766300
C	-0.22896800	1.36319700	1.73772500
C	1.86366200	2.31285400	1.48979900

C	-0.23750800	2.15245000	0.55007100
C	1.03001300	2.80375600	0.40993600
Zr	1.30764700	0.11251100	0.20489300
C	2.25903400	-1.11522100	2.12472300
C	1.31801200	-2.09813000	1.60480300
C	3.34426700	-1.06509800	1.16761100
C	1.81335500	-2.59729900	0.34003800
C	3.02232700	-1.88499000	0.06100700
Si	1.86984100	0.13547100	3.50186100
C	0.69018400	-0.48097600	4.83721000
C	3.39988700	0.72913000	4.42918400
C	1.16423400	-3.68446200	-0.33565100
C	0.13880900	-2.67397900	2.16233100
C	0.03657500	-4.21648900	0.27171300
C	-0.47262600	-3.71544100	1.49929100
C	-1.47767900	0.74583800	2.31883500
C	4.67897700	-0.37964800	1.29908500
C	1.68521200	-4.25042400	-1.60792000
C	1.50297300	3.85652000	-0.45158000
C	3.17717100	2.83545800	1.66256600
C	2.80257000	4.29579900	-0.24457300
C	3.62831500	3.79842500	0.79272000
C	0.63781600	4.56614300	-1.42901700
C	3.04724500	-4.56373500	-1.76820600
C	3.51365400	-5.12218300	-2.95761000
C	2.63203500	-5.37408900	-4.01126000
C	0.80669000	-4.52150600	-2.67264600
C	1.27658200	-5.07456000	-3.86397000
C	-0.30042100	3.89874400	-2.23166400
C	-1.08152700	4.59008100	-3.15744700
C	-0.94982700	5.97208500	-3.29544700
C	0.74814200	5.96268300	-1.57152500
C	-0.03314200	6.65534900	-2.49391000
C	1.67011500	0.38235900	-2.61067600
C	-0.64803700	-0.37621900	-1.98755800
C	-1.27890200	-1.16486200	-1.00471000
C	-2.63005800	-0.97000300	-0.68217600
C	-3.40079700	-0.01481600	-1.34629900
C	-1.43169600	0.58419100	-2.66785700
C	-2.77013800	0.74872800	-2.35496400
C	-4.87429900	0.20999400	-1.06704800
H	-1.11853400	2.33708500	-0.04925200
H	3.66423900	-2.03061600	-0.79668400
H	0.63793300	0.28528700	5.61942500

H	-0.33215200	-0.68260800	4.51640100
H	1.09012000	-1.38935200	5.30134500
H	3.18333100	1.65936900	4.96587300
H	3.65306900	-0.02741500	5.18094900
H	4.28908900	0.88508200	3.81766500
H	-0.22949600	-2.35357700	3.12885800
H	-0.45069500	-5.07207100	-0.18567400
H	-1.34088500	-4.19639000	1.93954700
H	3.78612200	2.52960300	2.50322900
H	3.19523800	5.07971500	-0.88381700
H	4.62101200	4.21945700	0.91905700
H	3.73583000	-4.40792200	-0.94373700
H	4.56567800	-5.37217400	-3.05704200
H	2.99795300	-5.80719100	-4.93701800
H	-0.24930300	-4.28841100	-2.56687800
H	0.58314300	-5.27161900	-4.67597500
H	-0.41311500	2.82665900	-2.14208900
H	-1.79296200	4.04890800	-3.77536600
H	-1.55917900	6.51202300	-4.01349700
H	1.43262400	6.51302200	-0.93401800
H	0.06745500	7.73308200	-2.57921700
H	-2.29759500	0.79642000	1.59954700
H	-1.35691800	-0.29910800	2.61019600
H	-1.78108600	1.30367600	3.21173000
H	5.22135800	-0.42784800	0.35175100
H	4.60288400	0.67025100	1.57831300
H	5.28096700	-0.89051100	2.05923800
H	1.38666300	1.42776300	-2.69605400
H	-0.74781200	-1.99295000	-0.54757400
H	-3.07971600	-1.60366100	0.07355200
H	-0.99099600	1.15190100	-3.48068200
H	-3.36156300	1.46900900	-2.91470200
H	1.11895100	-1.62828700	-2.29336700
H	2.68719800	0.13662900	-2.89160900
H	-5.01277400	1.26797200	-0.80161600
H	-5.42011000	0.08124000	-2.01224800
H	2.75116600	0.84921900	-0.60271100
C	-5.51899300	-0.66846000	0.01099900
H	-5.41131200	-1.72727200	-0.26180800
H	-4.98500400	-0.53423200	0.96002100
C	-7.00828800	-0.34693400	0.20197500
H	-7.51136000	-0.42880600	-0.77127800
H	-7.11664100	0.70285600	0.51210600
C	-7.74730500	-1.24644300	1.21299000

H	-7.60139000	-2.29086400	0.89774700
C	-7.19997900	-1.10144000	2.64166200
H	-7.75803200	-1.73555300	3.33806400
H	-6.14527400	-1.38672500	2.71625800
H	-7.29297500	-0.06582800	2.99153400
C	-9.25477000	-0.95331000	1.18255000
H	-9.67004800	-1.09081600	0.17847500
H	-9.79973400	-1.61472200	1.86364700
H	-9.45930000	0.07937900	1.48992700

TS3_{2,1}

C	0.86023100	-0.54925000	-2.19217800
C	1.06866000	1.40501300	2.31184900
C	-0.25308100	1.37493300	1.74644400
C	1.84557300	2.29934200	1.46458200
C	-0.26828700	2.16048200	0.55357600
C	1.00022800	2.80251700	0.39902300
Zr	1.23796100	0.08880000	0.19482700
C	2.25464800	-1.10470600	2.10193800
C	1.33369300	-2.11513600	1.59943200
C	3.32695000	-1.03168800	1.13023000
C	1.82550300	-2.60764600	0.33129300
C	3.01385400	-1.86694100	0.03441400
Si	1.86338600	0.13764200	3.48509400
C	0.69300300	-0.49132800	4.82240100
C	3.39598000	0.73535100	4.40606700
C	1.18880900	-3.70342700	-0.33934100
C	0.16470300	-2.70400800	2.16380300
C	0.07052300	-4.24918500	0.27396200
C	-0.43733200	-3.75367800	1.50385800
C	-1.49816700	0.75981100	2.33848300
C	4.65071600	-0.32021000	1.23959300
C	1.70836900	-4.25744400	-1.61721000
C	1.46942900	3.86059100	-0.46035300
C	3.16242800	2.81914700	1.62813500
C	2.77658500	4.28501000	-0.27197200
C	3.61218900	3.77828800	0.75380500
C	0.59373300	4.59711400	-1.40845100
C	3.07268100	-4.55606400	-1.78545400
C	3.53935000	-5.10152100	-2.98081800
C	2.65534000	-5.35445500	-4.03218900
C	0.82752500	-4.52937200	-2.67955400
C	1.29766300	-5.06912400	-3.87679100

C	-0.36728700	3.95546700	-2.20451300
C	-1.15758600	4.67244700	-3.10261300
C	-1.01243600	6.05516100	-3.21777800
C	0.71749400	5.99495200	-1.52698200
C	-0.07310700	6.71325700	-2.42134900
C	1.78410800	0.46566400	-2.39027000
C	-0.57363100	-0.34847800	-1.92503600
C	-1.21444100	-1.14746500	-0.95196600
C	-2.57635300	-0.96886600	-0.65224200
C	-3.34406600	-0.01786900	-1.32093000
C	-1.35942800	0.60959500	-2.60960700
C	-2.70330500	0.75673500	-2.31713300
C	-4.82380300	0.19416400	-1.06421000
H	-1.15567400	2.35193300	-0.03371800
H	3.65074700	-2.00720300	-0.82820200
H	0.63628600	0.27261600	5.60654600
H	-0.32834800	-0.70056500	4.50318300
H	1.10150500	-1.39742000	5.28347600
H	3.18255100	1.66783800	4.94005300
H	3.65156200	-0.01861900	5.15958100
H	4.28319500	0.88803200	3.79052800
H	-0.20519200	-2.38446400	3.13006600
H	-0.41035000	-5.10918900	-0.18183200
H	-1.29873600	-4.24334600	1.94800200
H	3.77412300	2.51601700	2.46771100
H	3.16542100	5.07145600	-0.91049300
H	4.60786100	4.19473200	0.87190000
H	3.76327100	-4.39868400	-0.96277800
H	4.59330000	-5.34052600	-3.08675900
H	3.02119700	-5.77730300	-4.96271200
H	-0.22987700	-4.30604400	-2.56782500
H	0.60271000	-5.26661500	-4.68738500
H	-0.48985200	2.88357300	-2.13223100
H	-1.88652000	4.15052100	-3.71658200
H	-1.62902300	6.61519500	-3.91393200
H	1.41973800	6.52584400	-0.89230300
H	0.03797600	7.79125500	-2.48844300
H	-2.32611500	0.82101100	1.62947700
H	-1.37820800	-0.28928000	2.61644500
H	-1.78822100	1.30916500	3.24085700
H	5.18950400	-0.37999000	0.29047800
H	4.56204700	0.73347300	1.49973100
H	5.26639900	-0.80692800	2.00445900
H	1.47035500	1.49733400	-2.52897000

H	-0.69336600	-1.99080600	-0.51053000
H	-3.03250700	-1.61531700	0.08872800
H	-0.91201500	1.18499000	-3.41319600
H	-3.29422700	1.47180600	-2.88435700
H	1.20335800	-1.57852300	-2.25103000
H	2.77286700	0.22895500	-2.76701800
H	-4.97322600	1.24580000	-0.77976900
H	-5.35271300	0.08118600	-2.02091200
H	2.56208100	0.83552300	-0.85425100
C	-5.48187200	-0.70878000	-0.01487500
H	-5.36384100	-1.76129200	-0.30719700
H	-4.96401300	-0.59135300	0.94529500
C	-6.97556200	-0.39835900	0.15902300
H	-7.46348500	-0.46363500	-0.82318000
H	-7.09399700	0.64464200	0.48783700
C	-7.72531500	-1.32072500	1.14114400
H	-7.57018200	-2.35810600	0.80762000
C	-7.19935400	-1.20185900	2.58026100
H	-7.76530800	-1.85120800	3.25595900
H	-6.14488600	-1.48522600	2.66460100
H	-7.30092000	-0.17357400	2.94888100
C	-9.23345200	-1.03339500	1.09454000
H	-9.63332400	-1.15255900	0.08191200
H	-9.78531500	-1.71055200	1.75429600
H	-9.44707200	-0.00790300	1.41933000

PR3_{2,1}

C	0.94610000	-0.46420000	-2.03749100
C	0.98895900	1.43699300	2.33193800
C	-0.33117400	1.36256800	1.77144000
C	1.74410800	2.32741900	1.45998600
C	-0.37330600	2.13768400	0.56853800
C	0.87487900	2.80844000	0.39930400
Zr	1.17583600	0.09340600	0.19148900
C	2.27872900	-1.01749500	2.08602600
C	1.41293400	-2.08104100	1.59154900
C	3.34158000	-0.89081700	1.10747900
C	1.92655400	-2.55322600	0.32483500
C	3.07033500	-1.74863300	0.01786300
Si	1.84376100	0.19188200	3.48651200
C	0.71222400	-0.50346700	4.82417700
C	3.35603600	0.84109500	4.40662200

C	1. 33878100	-3. 67193300	-0. 34706600
C	0. 26677900	-2. 71365700	2. 15238700
C	0. 23960500	-4. 26173500	0. 26279100
C	-0. 29093900	-3. 78737900	1. 48988900
C	-1. 56137400	0. 73018300	2. 37678400
C	4. 64106500	-0. 13302700	1. 21208900
C	1. 88349400	-4. 20153100	-1. 62427100
C	1. 31450600	3. 87691300	-0. 46715700
C	3. 04825200	2. 88611100	1. 61451700
C	2. 61837500	4. 31954400	-0. 30038700
C	3. 47416700	3. 84019800	0. 72418800
C	0. 41166800	4. 61160900	-1. 39105600
C	3. 25815100	-4. 45209400	-1. 78500000
C	3. 75042500	-4. 97458700	-2. 98037500
C	2. 88153500	-5. 25132100	-4. 03828600
C	1. 01820700	-4. 49684800	-2. 69268400
C	1. 51395500	-5. 01290700	-3. 88987700
C	-0. 56900100	3. 97021000	-2. 16262900
C	-1. 38537100	4. 68870400	-3. 03589700
C	-1. 24764600	6. 07223000	-3. 14946000
C	0. 52691100	6. 01090300	-1. 50592300
C	-0. 28961100	6. 73030700	-2. 37552600
C	1. 87425400	0. 66099900	-2. 29510500
C	-0. 49998900	-0. 33154100	-1. 88140800
C	-1. 12965500	-1. 14650300	-0. 90254700
C	-2. 50876200	-1. 02785000	-0. 63146900
C	-3. 30169200	-0. 11131800	-1. 31152300
C	-1. 32064900	0. 59721500	-2. 57211700
C	-2. 67291500	0. 68529800	-2. 30203600
C	-4. 79307900	0. 04524000	-1. 08026500
H	-1. 26870100	2. 29551400	-0. 01590900
H	3. 71052100	-1. 86413100	-0. 84644300
H	0. 61928300	0. 25185500	5. 61318500
H	-0. 29868500	-0. 76384400	4. 50883300
H	1. 16924400	-1. 38984300	5. 27798600
H	3. 10792000	1. 75896100	4. 95089100
H	3. 64379200	0. 09026100	5. 15153700
H	4. 23500800	1. 03562500	3. 79081500
H	-0. 12056800	-2. 40453100	3. 11489800
H	-0. 20717300	-5. 13794600	-0. 19669100
H	-1. 13578200	-4. 30862500	1. 92978500
H	3. 66602700	2. 61537800	2. 46048700
H	2. 98524000	5. 11002000	-0. 94679200
H	4. 46047300	4. 28106700	0. 83168500

H	3.93793300	-4.27519800	-0.95702400
H	4.81251500	-5.17693900	-3.08130500
H	3.26700000	-5.65616900	-4.96891100
H	-0.04626500	-4.30734300	-2.58683700
H	0.83123400	-5.22826700	-4.70626000
H	-0.68613100	2.89816900	-2.09234700
H	-2.12951000	4.16658200	-3.63103100
H	-1.88490500	6.63316100	-3.82602600
H	1.24208900	6.54262100	-0.88663400
H	-0.18458400	7.80907100	-2.43999300
H	-2.38084100	0.72787000	1.65560200
H	-1.40766900	-0.29943900	2.70524600
H	-1.88307500	1.31006500	3.24898800
H	5.17691700	-0.16848900	0.25960200
H	4.52516100	0.91389500	1.48641600
H	5.27805400	-0.60878100	1.96630900
H	1.42770900	1.57853900	-2.68613600
H	-0.59778000	-1.99570100	-0.48381000
H	-2.95127800	-1.69603900	0.09880200
H	-0.88862600	1.19221700	-3.36994000
H	-3.28499600	1.37068000	-2.88399000
H	1.32346400	-1.46679100	-2.20675600
H	2.75126000	0.38716300	-2.88504200
H	-4.98789100	1.08770500	-0.78909400
H	-5.30256600	-0.07993300	-2.04598500
C	-5.43375000	-0.89041300	-0.04886100
H	-5.27388800	-1.93512300	-0.34932400
H	-4.93305900	-0.76450900	0.91939200
C	-6.93961400	-0.63588700	0.10898400
H	-7.41336800	-0.71012100	-0.87950100
H	-7.09982300	0.39918200	0.44512000
C	-7.66675700	-1.59337600	1.07449300
H	-7.46642700	-2.62163800	0.73679400
C	-7.16572700	-1.46396300	2.52163200
H	-7.71337200	-2.14115800	3.18505400
H	-6.10161900	-1.70394700	2.61825000
H	-7.31479800	-0.44349200	2.89576600
C	-9.18427800	-1.36541500	1.00860000
H	-9.56515100	-1.49533600	-0.01001300
H	-9.71808200	-2.06695900	1.65772300
H	-9.44278500	-0.35069500	1.33455300
H	2.38877700	1.03658900	-1.30881500

[IM3_{1,2}]

C	-10.44306800	1.18386800	0.30717200
C	5.48806800	-1.47436900	0.96954900
C	5.51424200	-1.54926500	-0.47255000
C	4.33417000	-2.26400400	1.38321400
C	4.36624400	-2.24858200	-0.92507800
C	3.64644600	-2.75465600	0.20855500
Zr	3.59376400	-0.08548400	0.23317200
C	5.07583800	1.19474400	1.72853400
C	5.04049100	2.02413200	0.53263500
C	3.76695500	1.32725800	2.33236800
C	3.72347200	2.61531500	0.40469300
C	2.94125600	2.11329700	1.49378600
Si	6.35701900	-0.17481300	2.05901900
C	8.10788700	0.22965900	1.48859400
C	6.51169200	-0.64427300	3.87709200
C	3.44194100	3.57807300	-0.62529500
C	6.04505800	2.35967500	-0.42108400
C	4.46137500	3.85257700	-1.52375600
C	5.74122600	3.24788500	-1.42923600
C	6.58759500	-1.06770500	-1.41840800
C	3.29571500	0.81418500	3.66872300
C	2.14532900	4.29894900	-0.71187700
C	2.51664200	-3.62980400	0.32422700
C	3.85113500	-2.62632500	2.67025500
C	2.10158300	-3.94988000	1.60947000
C	2.75327000	-3.45502900	2.76233500
C	1.85154800	-4.24248000	-0.85394400
C	1.51067600	4.80760500	0.43622300
C	0.31545100	5.51853700	0.33592100
C	-0.27394000	5.73543700	-0.91167700
C	1.54613000	4.53716900	-1.96308700
C	0.34805200	5.24484400	-2.06167400
C	2.59310100	-4.76342200	-1.93053300
C	1.95551900	-5.38428100	-3.00502000
C	0.56478000	-5.50273700	-3.02613100
C	0.45119900	-4.37771900	-0.88539300
C	-0.18443000	-5.00206400	-1.95878300
C	-11.32129900	-0.02668700	0.68864500
C	-12.76907900	0.36625100	1.00933500
C	-13.71387400	-0.81295400	1.31868200
C	-9.01474200	0.79795100	-0.00859200
C	-8.04898600	0.70935200	1.00356900
C	-6.74615300	0.30009200	0.72295900
C	-6.36174900	-0.03422800	-0.58199100

C	-8.62583800	0.46761300	-1.31358000
C	-7.32280500	0.05852400	-1.59611200
C	-15.16485600	-0.32201300	1.43344300
H	2.03652700	-0.55617400	1.05234000
H	4.16098500	-2.47520800	-1.96270700
H	1.91175000	2.36017500	1.71114200
H	8.77119400	-0.57844100	1.81785600
H	8.24365200	0.34084100	0.41221700
H	8.45284400	1.15022300	1.97251400
H	7.03597600	-1.60171300	3.97218700
H	7.12664100	0.11372900	4.37580200
H	5.57387100	-0.71237200	4.42893400
H	7.05417400	1.98328700	-0.31115300
H	4.29858000	4.60460600	-2.28938100
H	6.51048400	3.53990000	-2.13762200
H	4.38020700	-2.32109400	3.56419800
H	1.27938700	-4.64679400	1.73617900
H	2.40024100	-3.77099200	3.73913600
H	1.97679300	4.68325900	1.40807000
H	-0.14894100	5.91594100	1.23348700
H	-1.20312500	6.29182200	-0.98786500
H	2.01850300	4.15721000	-2.86480000
H	-0.09723100	5.41431400	-3.03748100
H	3.67737400	-4.72793700	-1.90475700
H	2.54873800	-5.79237900	-3.81792400
H	0.07015300	-5.99049400	-3.86037400
H	-0.14022200	-3.97953700	-0.06618900
H	-1.26620300	-5.10012200	-1.96012600
H	6.29703700	-1.26804600	-2.45354300
H	6.80313400	-0.00125300	-1.33730300
H	7.52060500	-1.60864800	-1.22836800
H	2.22609200	1.00287300	3.78691000
H	3.45393900	-0.25535000	3.80692500
H	3.82378700	1.33842300	4.47317900
H	-10.86312100	-0.53505700	1.54545900
H	-12.77813400	1.06328200	1.86075100
H	-13.17785500	0.92641200	0.15663000
H	-8.32323300	0.95958600	2.02575000
H	-6.02016700	0.23280200	1.53071900
H	-9.35432700	0.52756300	-2.11867900
H	-7.05210000	-0.19804400	-2.61822600
H	-10.88754900	1.69085800	-0.55831700
H	-11.30938600	-0.75047000	-0.13759300
C	-13.30354700	-1.57968400	2.58544900

H	-15.85265500	-1.15536000	1.61219300
H	-15.27547100	0.38257200	2.26685400
H	-15.48863400	0.18972300	0.52056100
H	-13.66207100	-1.51123300	0.46934000
H	-13.99882900	-2.40178500	2.78585400
H	-12.30108900	-2.01094300	2.50296800
H	-13.31286200	-0.91837000	3.46094100
C	1.59623500	-0.34284900	-2.10001100
H	1.79145200	-1.39215900	-2.32201100
C	2.67439500	0.50966600	-2.09250500
H	-10.45549200	1.90756500	1.13194700
H	3.61085300	0.16211800	-2.53148000
H	2.54417800	1.58487500	-2.03046800
C	0.20507100	-0.03480400	-1.84945400
C	-0.73628300	-1.08089300	-1.92997700
C	-0.26522200	1.26500900	-1.55084500
C	-2.08911300	-0.84578800	-1.71373000
H	-0.39728200	-2.08582500	-2.16262800
C	-1.61333200	1.48745000	-1.33140900
H	0.42332600	2.10076900	-1.49262800
C	-2.55711300	0.44083200	-1.40730700
H	-2.78479800	-1.67428200	-1.78308400
H	-1.95382100	2.49316800	-1.10061500
C	-4.02170200	0.74844600	-1.17794400
H	-4.10126300	1.46586900	-0.35169200
H	-4.40541200	1.28355400	-2.05856800
C	-4.94001700	-0.45556600	-0.88994700
H	-4.94462700	-1.13025600	-1.75397800
H	-4.53124300	-1.02424300	-0.04560200

[TS3_{1,2}]

C	10.60222300	-0.37196200	1.60064800
C	-5.54874500	0.65258500	1.44922100
C	-6.01455000	0.70466100	0.08150800
C	-4.56749300	1.72489000	1.56712500
C	-5.27635300	1.68485000	-0.63389300
C	-4.41729000	2.37767600	0.28161100
Zr	-3.63977100	-0.14640100	0.11230200
C	-4.23000400	-1.81441000	1.82817200
C	-4.37544500	-2.54302900	0.57350900
C	-2.80732200	-1.61154100	1.99471100
C	-3.06815500	-2.72487900	-0.02661600
C	-2.12405900	-2.09890300	0.84985800

Si	-5.65471500	-0.83678100	2.64016900
C	-7.32661400	-1.70668800	2.61013000
C	-5.33797000	-0.42076500	4.45083700
C	-2.91481600	-3.46694000	-1.24969200
C	-5.51857700	-3.09839700	-0.07478100
C	-4.06864900	-3.94998800	-1.84303800
C	-5.35247100	-3.77244300	-1.26296600
C	-7.17108200	-0.03325700	-0.54638000
C	-2.07691300	-1.04389400	3.18654100
C	-1.58432000	-3.77116200	-1.83593100
C	-3.56852800	3.52423000	0.12720000
C	-3.81429200	2.20480400	2.67676200
C	-2.87853000	3.95116900	1.25360000
C	-2.99473600	3.30088400	2.50550300
C	-3.45171200	4.25527700	-1.16058700
C	-0.53490800	-4.26297300	-1.03991400
C	0.69133100	-4.60333200	-1.61057700
C	0.89697600	-4.44894900	-2.98387700
C	-1.36740300	-3.62987800	-3.21868800
C	-0.13649400	-3.96005100	-3.78618000
C	-4.58569800	4.56911000	-1.93196600
C	-4.46151800	5.27862300	-3.12569200
C	-3.20375000	5.68527500	-3.57656300
C	-2.19361700	4.68715500	-1.61912500
C	-2.07027900	5.39015100	-2.81720800
C	11.49958300	0.12838400	0.44926700
C	12.98990600	-0.13532000	0.70085900
C	13.92931300	0.24929400	-0.45988500
C	9.13131100	-0.11234000	1.36110300
C	8.32719900	-1.04586700	0.70000100
C	6.97691600	-0.79202800	0.44399600
C	6.38237100	0.40961000	0.84308400
C	8.53312700	1.09240600	1.76068100
C	7.18907000	1.34707300	1.50643700
C	15.36022100	-0.23047800	-0.17339600
H	-2.04997800	0.77774500	0.38636400
H	-5.44951100	1.95008700	-1.66784600
H	-1.05152600	-2.06618900	0.71388600
H	-8.02501500	-1.12276500	3.22057900
H	-7.78340500	-1.82743200	1.62731500
H	-7.24091600	-2.69674700	3.07156800
H	-6.04981500	0.34038400	4.78908000
H	-5.52145500	-1.32381200	5.04445300
H	-4.33154000	-0.07659800	4.69113900

H	-6.49262000	-3.05243000	0.39480400
H	-3.98364600	-4.54423800	-2.74734200
H	-6.21151500	-4.22616400	-1.74776800
H	-3.93956100	1.76549700	3.65823300
H	-2.26375400	4.84321700	1.18367600
H	-2.45169500	3.70137100	3.35605600
H	-0.69255700	-4.41572700	0.02322400
H	1.48281700	-5.00234900	-0.98313600
H	1.85126900	-4.71683800	-3.42706200
H	-2.16743000	-3.25313900	-3.85004400
H	0.01314400	-3.83965100	-4.85487900
H	-5.57272800	4.29425700	-1.57385000
H	-5.35046700	5.52495600	-3.69859700
H	-3.10906700	6.23526300	-4.50766300
H	-1.30462500	4.46358000	-1.03558000
H	-1.08886500	5.70800900	-3.15596800
H	-7.18031600	0.12122600	-1.62888900
H	-7.16334300	-1.10717400	-0.36550500
H	-8.11250700	0.36215600	-0.14876400
H	-1.01404100	-0.93216000	2.95867000
H	-2.44814100	-0.06895600	3.50533000
H	-2.16875900	-1.72800000	4.03735800
H	11.31882800	1.20011100	0.30364500
H	13.30699300	0.39915000	1.60886900
H	13.12499500	-1.20429800	0.91816900
H	8.75960900	-1.99154800	0.38131000
H	6.39539100	-1.55067200	-0.07057100
H	9.12994700	1.83776500	2.28121800
H	6.75378200	2.28989900	1.83167900
H	10.76761700	-1.44747200	1.74162100
H	11.18963600	-0.36284100	-0.48325300
C	13.91613000	1.75727400	-0.75429000
H	16.03049300	-0.00151300	-1.00876100
H	15.76633800	0.25948000	0.72009500
H	15.39394200	-1.31219400	-0.00316200
H	13.57407100	-0.27394600	-1.36086300
H	14.59927100	2.00084100	-1.57500800
H	12.92171500	2.11547200	-1.03798300
H	14.23965000	2.32831000	0.12501100
C	-1.49535200	0.88541000	-1.24152900
H	-1.69725900	1.95280200	-1.19227100
C	-2.43201900	0.11548700	-1.96388600
H	10.91392200	0.11482400	2.53341100
H	-3.13978300	0.66111500	-2.58547000

H	-2.14709500	-0.86820700	-2.32745300
C	-0.08626700	0.54405600	-0.95973300
C	0.69292500	1.45368600	-0.22554200
C	0.53232300	-0.62337200	-1.44050300
C	2.03730200	1.20624100	0.03386200
H	0.23261300	2.36182900	0.15648800
C	1.87630400	-0.86325000	-1.17873900
H	-0.02318700	-1.33695800	-2.03869000
C	2.65797400	0.03859800	-0.43583500
H	2.60469200	1.93342900	0.60351600
H	2.33361800	-1.76915500	-1.56716800
C	4.11876900	-0.28822800	-0.18780200
H	4.16408400	-1.25846100	0.32495700
H	4.60143800	-0.45144200	-1.16067400
C	4.91735300	0.74594800	0.60849100
H	4.86244200	1.71531500	0.09484200
H	4.43446200	0.89907400	1.58379700

[PR3_{1,2}]

C	10.76952400	-1.03977200	0.14570100
C	-6.12713800	0.98516700	0.01625200
C	-5.63833200	1.28246600	-1.31522700
C	-5.36520400	1.85215700	0.91000800
C	-4.54989500	2.18190500	-1.23009700
C	-4.37824300	2.57990000	0.13784200
Zr	-3.86574100	0.02381500	-0.04228900
C	-5.44441200	-1.64043100	0.78675800
C	-4.73338300	-2.30199900	-0.30631700
C	-4.48953200	-1.55756800	1.87124300
C	-3.37527900	-2.58502400	0.11354800
C	-3.23062900	-2.03528900	1.43300800
Si	-7.03173800	-0.59413900	0.59583400
C	-8.26042300	-1.26460800	-0.66456800
C	-8.00429500	-0.39800700	2.19731600
C	-2.47889300	-3.33383900	-0.70983700
C	-5.12123000	-2.64426800	-1.63074000
C	-2.92871500	-3.66334600	-1.98501600
C	-4.21599300	-3.30699300	-2.44247800
C	-6.17051100	0.78023700	-2.63418600
C	-4.72680400	-1.15427200	3.30462100
C	-1.15655400	-3.79600800	-0.22322200
C	-3.48471600	3.51701400	0.76307200
C	-5.45824800	2.09544000	2.31064400

C	-3.60687700	3.67865400	2.13439600
C	-4.58635700	2.98862800	2.89455000
C	-2.49887200	4.30778700	-0.01731600
C	-1.02092400	-4.37732600	1.05090800
C	0.21140200	-4.86487400	1.48256700
C	1.33130300	-4.77633700	0.65323600
C	-0.02353600	-3.72299900	-1.05159000
C	1.20947600	-4.20314900	-0.61393000
C	-2.86871000	4.97058900	-1.20143800
C	-1.94108100	5.73698900	-1.90637800
C	-0.62745600	5.85078500	-1.44627300
C	-1.17625600	4.44171200	0.44177400
C	-0.24863400	5.20286200	-0.26884800
C	11.67014600	0.21327600	0.14115200
C	13.16253400	-0.12726700	0.24441900
C	14.11758100	1.08109100	0.16680100
C	2.70571500	-0.53967700	-0.38582000
C	1.91048100	-0.32558500	0.74670900
C	0.57345200	0.05543500	0.62661100
C	-0.01119700	0.23058800	-0.63176600
C	2.11108700	-0.36715500	-1.64477900
C	0.77574200	0.00878500	-1.77043500
C	15.57647700	0.60745800	0.08401300
H	-4.00311900	2.57004400	-2.07732600
H	-2.34984300	-2.11429600	2.05652400
H	-9.15757400	-0.63542000	-0.63895700
H	-7.91776300	-1.29573200	-1.69914300
H	-8.56516500	-2.27719600	-0.37753100
H	-8.74667600	0.39954700	2.08154600
H	-8.55253200	-1.32877500	2.38286700
H	-7.41651400	-0.18637200	3.09093500
H	-6.13328900	-2.47231700	-1.97555300
H	-2.28857600	-4.25598400	-2.63057300
H	-4.51959700	-3.61031900	-3.43987300
H	-6.24743100	1.64080900	2.89589500
H	-2.97322200	4.40423300	2.63453800
H	-4.67225700	3.20594600	3.95481300
H	-1.89318400	-4.48859900	1.68782900
H	0.29371300	-5.32671000	2.46191800
H	2.29094500	-5.15601300	0.99036900
H	-0.10365100	-3.26460900	-2.03239600
H	2.07595600	-4.12749200	-1.26342600
H	-3.89625100	4.92015200	-1.54847400
H	-2.24826400	6.25525500	-2.80976700

H	0.09387800	6.44587000	-1.99763700
H	-0.87234000	3.93643500	1.35433300
H	0.76984300	5.28871900	0.09738600
H	-5.55916400	1.15791300	-3.45723300
H	-6.19185800	-0.30799900	-2.71247100
H	-7.19412300	1.14061900	-2.78160200
H	-3.77730700	-1.08326400	3.84197700
H	-5.24431700	-0.20370300	3.41862400
H	-5.33067700	-1.92254400	3.80044000
H	11.36707700	0.86512900	0.96926200
H	13.34914000	-0.66928600	1.18376500
H	13.41923300	-0.82724800	-0.56320100
H	2.34089600	-0.46013100	1.73577700
H	-0.01747200	0.21939600	1.52628400
H	2.70464200	-0.52957800	-2.54126300
H	0.34265100	0.13828300	-2.75866000
H	11.48398000	0.78311700	-0.77937900
C	13.93354000	2.05328400	1.34236400
H	16.26401500	1.45444300	-0.01326200
H	15.86026900	0.05334500	0.98717500
H	15.73555000	-0.05353600	-0.77497500
H	13.88829600	1.62619300	-0.76161800
H	14.63254200	2.89308900	1.26724500
H	12.92257400	2.47055000	1.38082600
H	14.12426100	1.54898400	2.29800900
C	-1.43753900	0.72477300	-0.79425200
H	-1.44153900	1.79153000	-1.04094800
C	-2.37312800	-0.04604600	-1.71834400
H	-2.62575100	0.49872100	-2.62752600
H	-2.01257400	-1.04707000	-1.95686300
H	-1.83768400	0.73998300	0.28956500
C	4.17024300	-0.89328100	-0.26045400
H	4.34458000	-1.45308200	0.66522000
H	4.46903300	-1.55046100	-1.08523000
C	5.08800100	0.35861400	-0.26743700
H	4.79528900	1.01232200	0.56290200
H	4.90228400	0.92345400	-1.18883100
C	6.55634100	0.01015700	-0.16057300
C	7.18321200	-0.10233200	1.08708300
C	7.32203500	-0.24539800	-1.30548000
C	8.52858100	-0.45549500	1.18584200
H	6.61325600	0.09374600	1.99300000
C	8.66723400	-0.59846000	-1.20572100
H	6.86188800	-0.16198800	-2.28794900

C	9.29686700	-0.70887900	0.04145500
H	8.99146700	-0.53330700	2.16692600
H	9.23964200	-0.78875900	-2.11068000
H	11.05959200	-1.69237800	-0.68735900
H	10.95533300	-1.60875300	1.06543500

[IM3_{2,1}]

C	2.30247800	-0.65700600	-2.26420500
C	2.69851800	1.68233800	2.19827900
C	1.35916000	1.38035400	1.76348900
C	3.21846400	2.65205600	1.24684900
C	1.09877800	2.07199400	0.54371900
C	2.21274300	2.91813500	0.23693800
Zr	2.93872400	0.31273500	0.13951900
C	4.25958100	-0.61136500	2.01261200
C	3.45322900	-1.76772800	1.64717300
C	5.22416600	-0.44978700	0.94515200
C	3.89994700	-2.26215300	0.36293000
C	4.93998600	-1.38393800	-0.07811300
Si	3.79897000	0.65045900	3.35627200
C	2.87841600	-0.06248100	4.83929700
C	5.28742200	1.55235400	4.07954400
C	3.37810500	-3.48197800	-0.18518300
C	2.45083400	-2.49066400	2.35769600
C	2.42141000	-4.14852400	0.56572000
C	1.96035800	-3.65870100	1.81643600
C	0.30091000	0.59364400	2.49783800
C	6.43069100	0.45134200	0.89916800
C	3.85546400	-4.03862300	-1.47861900
C	2.41014000	3.97286900	-0.72368900
C	4.43136900	3.39886800	1.25128400
C	3.62568100	4.63999900	-0.67766000
C	4.62129700	4.36210200	0.29027200
C	1.34458300	4.45442800	-1.64004000
C	5.22727500	-4.13881300	-1.77375200
C	5.65684900	-4.69151200	-2.97967500
C	4.72727200	-5.14984200	-3.91595900
C	2.93090600	-4.51574100	-2.42566100
C	3.36290000	-5.06252000	-3.63405600
C	0.46990400	3.58133100	-2.30510200
C	-0.50790000	4.06211200	-3.17563200
C	-0.64098900	5.43350800	-3.39456100
C	1.18865900	5.83596200	-1.86279600

C	0.21077500	6.31823100	-2.73012500
C	2.98337200	0.42857500	-2.71848100
C	0.89322500	-0.65223400	-1.82674800
C	0.49002000	-1.44846900	-0.73617300
C	-0.84432800	-1.45417800	-0.30233300
C	-1.81952100	-0.70059700	-0.95737700
C	-0.09566200	0.10841200	-2.49164500
C	-1.41261400	0.07424300	-2.06724800
C	-9.47648800	-1.23906900	1.50652700
H	0.14706100	2.05947100	0.02992400
H	5.51176500	-1.48174600	-0.99047000
H	2.78305500	0.72992900	5.59063800
H	1.87484000	-0.43833800	4.63904500
H	3.46425400	-0.86965200	5.29272000
H	4.96759500	2.46539900	4.59376900
H	5.74331100	0.89911900	4.83266700
H	6.06967200	1.81645500	3.36742800
H	2.13460800	-2.17226800	3.34296700
H	2.04181400	-5.09942900	0.20477500
H	1.23442200	-4.24480900	2.37180500
H	5.16269800	3.25775400	2.03633400
H	3.81164600	5.43321900	-1.39432500
H	5.53269700	4.95203400	0.28823900
H	5.96048000	-3.82110900	-1.03910300
H	6.72020700	-4.77513100	-3.18320900
H	5.06448700	-5.57804900	-4.85480200
H	1.86700200	-4.44809800	-2.21536400
H	2.63316600	-5.42052600	-4.35403400
H	0.56216800	2.51443200	-2.15191300
H	-1.16594000	3.36484300	-3.68706600
H	-1.40367800	5.80972400	-4.06925100
H	1.82113300	6.53859600	-1.32972800
H	0.10741900	7.38877200	-2.87909200
H	-0.58602400	0.47618900	1.87186600
H	0.62564600	-0.40367200	2.80047800
H	0.00239000	1.13332900	3.40330900
H	6.88731600	0.41708400	-0.09298200
H	6.20447800	1.49421100	1.11731100
H	7.17551100	0.10632800	1.62535800
H	2.51867500	1.40372600	-2.83597400
H	1.19157000	-2.13376400	-0.27168000
H	-1.11455100	-2.08706100	0.53558100
H	0.17390500	0.67416700	-3.37738900
H	-2.16248400	0.63862400	-2.61587100

H	2.81358200	-1.61706100	-2.23565800
H	3.99893400	0.33456900	-3.08417100
H	4.15075000	1.22278700	-0.85016300
C	-10.15196100	-0.34377400	0.44626300
H	-9.70191200	0.65781000	0.48590700
H	-9.92064800	-0.74287900	-0.54863600
C	-11.66992000	-0.23649400	0.64084500
H	-11.86929900	0.09162500	1.67070700
H	-12.12032600	-1.23628300	0.55013200
C	-12.38921700	0.72515200	-0.32645500
H	-11.90899400	1.71125700	-0.23227300
C	-12.27294700	0.28248700	-1.79320700
H	-12.80721300	0.97439900	-2.45300700
H	-11.23324000	0.24253000	-2.13294900
H	-12.71013400	-0.71369500	-1.93610600
C	-13.86409200	0.88176500	0.07319500
H	-13.96481000	1.23784000	1.10424400
H	-14.37884400	1.59470800	-0.57958300
H	-14.39318700	-0.07622300	-0.00095600
C	-3.28506400	-0.70686100	-0.57109000
H	-3.59684900	0.32681700	-0.36906900
H	-3.86930600	-1.01213400	-1.44941500
C	-3.68922500	-1.59130500	0.62249200
H	-3.39656000	-2.62947200	0.42362200
H	-3.14101300	-1.27208400	1.51819300
C	-5.17936800	-1.52725000	0.88765500
C	-6.05669100	-2.43611300	0.28315200
C	-5.72300300	-0.53490500	1.71285200
C	-7.43252100	-2.35135700	0.49335300
H	-5.65988300	-3.22584800	-0.35139800
C	-7.09919200	-0.45143400	1.92150200
H	-5.06298200	0.17532400	2.20705200
C	-7.98062900	-1.35592600	1.31367300
H	-8.09135200	-3.07529100	0.01987300
H	-7.49571900	0.32265000	2.57412500
H	-9.93057400	-2.23728700	1.47277000
H	-9.68861000	-0.83517500	2.50428900

[TS3_{2,1}]

C	2.63116400	-0.63440000	-2.09342900
C	2.64151800	1.34532200	2.40455900
C	1.35633600	1.37358400	1.75810800
C	3.51119600	2.19782200	1.60411300

C	1.45257700	2.15167500	0.56209400
C	2.75830500	2.73324600	0.48453200
Zr	2.88167300	0.01169400	0.30261900
C	3.72180100	-1.21406400	2.27529400
C	2.78879700	-2.18783900	1.72220800
C	4.85638100	-1.19941300	1.37242700
C	3.33401300	-2.71147800	0.48776500
C	4.57288100	-2.02810100	0.26193100
Si	3.30446600	0.05159400	3.63158400
C	2.02758700	-0.51938200	4.89647100
C	4.80282500	0.59270500	4.64169800
C	2.68866100	-3.78131500	-0.21686600
C	1.56322700	-2.72142900	2.21878200
C	1.50993600	-4.27159000	0.32932500
C	0.95310700	-3.74714000	1.52660300
C	0.04750500	0.82266200	2.27251900
C	6.20452900	-0.55251800	1.56182300
C	3.25823600	-4.36820000	-1.45898700
C	3.33042800	3.76315000	-0.34747300
C	4.83893500	2.65557600	1.84881700
C	4.64215400	4.12885000	-0.07681600
C	5.38757000	3.58918100	1.00189300
C	2.55214100	4.53188700	-1.35432900
C	4.61674600	-4.72742400	-1.54444500
C	5.12863000	-5.30549000	-2.70692700
C	4.29655900	-5.53180300	-3.80733400
C	2.42927100	-4.61312600	-2.57004400
C	2.94469100	-5.18605400	-3.73412300
C	1.61314300	3.92841000	-2.20642400
C	0.91284000	4.67423600	-3.15602200
C	1.12872800	6.04916700	-3.26913000
C	2.74864400	5.92251700	-1.47283000
C	2.04817100	6.66988900	-2.41898700
C	3.61523300	0.33320800	-2.24361400
C	1.19354400	-0.36173200	-1.92373300
C	0.45117800	-1.11783700	-0.98732700
C	-0.91974500	-0.87456300	-0.78496400
C	-1.59597800	0.10118800	-1.51660900
C	0.50218000	0.62509300	-2.66830200
C	-0.85174100	0.83599800	-2.47202300
C	-9.58930400	0.79357900	-0.51571300
H	0.61339700	2.38155600	-0.07978000
H	5.25512000	-2.20347700	-0.55846400
H	1.96595900	0.24308500	5.68199100

H	1. 01678400	-0. 67160000	4. 51606200
H	2. 35951600	-1. 44844800	5. 37361300
H	4. 60060700	1. 54528700	5. 14427000
H	4. 97445900	-0. 15671300	5. 42339300
H	5. 73363300	0. 69174800	4. 08191900
H	1. 15257200	-2. 38161200	3. 16140200
H	1. 01833700	-5. 11171700	-0. 15161800
H	0. 04604100	-4. 19556700	1. 92084300
H	5. 38023400	2. 32778500	2. 72655900
H	5. 10744200	4. 89209800	-0. 69220900
H	6. 39258200	3. 95905500	1. 18107200
H	5. 26434600	-4. 59254200	-0. 68353900
H	6. 17560100	-5. 59101400	-2. 74885700
H	4. 69723000	-5. 98043900	-4. 71120900
H	1. 37778100	-4. 34289900	-2. 52308400
H	2. 29024500	-5. 36214000	-4. 58264000
H	1. 43711100	2. 86361400	-2. 13770900
H	0. 19912600	4. 18146700	-3. 81077300
H	0. 58254700	6. 63172500	-4. 00466700
H	3. 43416700	6. 42613400	-0. 79862200
H	2. 21326800	7. 74115500	-2. 48491300
H	-0. 73078900	0. 92228500	1. 51280900
H	0. 09545800	-0. 23020700	2. 55977400
H	-0. 27078800	1. 39038500	3. 15412500
H	6. 79199900	-0. 62912200	0. 64300100
H	6. 15290400	0. 50160500	1. 83018800
H	6. 75346500	-1. 07590000	2. 35338600
H	3. 36324400	1. 37663000	-2. 41641000
H	0. 90074000	-1. 97674400	-0. 49916800
H	-1. 45425000	-1. 49241700	-0. 07189200
H	1. 02951600	1. 16926600	-3. 44507900
H	-1. 36895400	1. 56900300	-3. 08653800
H	2. 92699000	-1. 67934900	-2. 12488100
H	4. 61322400	0. 04239200	-2. 55238600
H	4. 30411100	0. 68870300	-0. 66325900
C	-10. 44194800	-0. 22095300	0. 27728800
H	-10. 29762300	-1. 22213800	-0. 15202900
H	-10. 06216300	-0. 27122700	1. 30505000
C	-11. 93592800	0. 13261200	0. 27368900
H	-12. 26621400	0. 25042500	-0. 76838400
H	-12. 07943600	1. 11472700	0. 74935600
C	-12. 85503100	-0. 89636900	0. 96464100
H	-12. 67846000	-1. 87286300	0. 48754400
C	-12. 55312900	-1. 04213100	2. 46528800

H	-13.23385600	-1.76254400	2.93195000
H	-11.53141700	-1.38883400	2.65065600
H	-12.68084900	-0.08295500	2.98331700
C	-14.33094400	-0.52657100	0.74568300
H	-14.57304000	-0.45768500	-0.32084200
H	-14.99766200	-1.27147800	1.19362000
H	-14.56287800	0.44334200	1.20326900
C	-3.07901000	0.38283800	-1.37078500
H	-3.20713300	1.40589400	-0.98968200
H	-3.52767700	0.39469800	-2.37267800
C	-3.88321900	-0.58337400	-0.47954100
H	-3.74124300	-1.61001700	-0.84033900
H	-3.49415300	-0.54993500	0.54608400
C	-5.36055000	-0.24506400	-0.47086100
C	-5.90106100	0.61524100	0.49414000
C	-6.21790400	-0.75164900	-1.45791200
C	-7.25388700	0.95947900	0.47121400
H	-5.25940100	1.01992800	1.27448100
C	-7.56957300	-0.40648700	-1.47928100
H	-5.82563300	-1.42577300	-2.21682100
C	-8.11384200	0.45602900	-0.51568100
H	-7.64867200	1.62914000	1.23174400
H	-8.21341000	-0.81329700	-2.25558200
H	-9.95685100	0.83762800	-1.54892900
H	-9.73807400	1.79393000	-0.08975800

[PR3_{2,1}]

C	2.73395800	-0.55231300	-1.94662400
C	2.54419100	1.36166200	2.41616100
C	1.26213200	1.35978700	1.76857800
C	3.40613200	2.20037000	1.59390200
C	1.34492500	2.13000300	0.56488100
C	2.63852900	2.72609300	0.47685200
Zr	2.80355900	-0.00358100	0.29675500
C	3.69849800	-1.16671700	2.26830500
C	2.80411700	-2.17858100	1.71971100
C	4.83353400	-1.11699300	1.36689900
C	3.37487300	-2.69573100	0.49578300
C	4.58683900	-1.96872300	0.26704800
Si	3.24620900	0.07885000	3.63072600
C	1.99690800	-0.54014600	4.89955300
C	4.73228600	0.65149800	4.64082800
C	2.76532900	-3.78036500	-0.21123600

C	1. 58189100	-2. 73081400	2. 19950300
C	1. 58848100	-4. 29131300	0. 32007800
C	1. 00368000	-3. 77197500	1. 50332400
C	-0. 04060100	0. 80557000	2. 29248400
C	6. 16477300	-0. 43346800	1. 55396600
C	3. 36390800	-4. 35511500	-1. 44406600
C	3. 19658600	3. 76402700	-0. 35859100
C	4. 72969200	2. 67885000	1. 83152900
C	4. 51313300	4. 12363000	-0. 11058000
C	5. 27079500	3. 59744000	0. 96703700
C	2. 39947900	4. 55677000	-1. 33099400
C	4. 72767200	-4. 69374000	-1. 50559900
C	5. 26879900	-5. 25669000	-2. 66080300
C	4. 46085600	-5. 48735800	-3. 77648700
C	2. 55916000	-4. 60453600	-2. 57000400
C	3. 10422800	-5. 16169900	-3. 72663900
C	1. 41746000	3. 98536100	-2. 15421300
C	0. 69956900	4. 75822500	-3. 06672300
C	0. 93954000	6. 12843800	-3. 17004200
C	2. 61800200	5. 94466500	-1. 43685100
C	1. 90029900	6. 71825700	-2. 34614500
C	3. 74561000	0. 51548900	-2. 11258600
C	1. 29210500	-0. 32956800	-1. 90128800
C	0. 53986700	-1. 10179800	-0. 97512200
C	-0. 84717600	-0. 89884500	-0. 81244300
C	-1. 52671500	0. 06269000	-1. 55047200
C	0. 58697600	0. 64836500	-2. 64920300
C	-0. 77422700	0. 81823800	-2. 48606000
C	-9. 52676300	0. 69774900	-0. 57262100
H	0. 50172300	2. 33318100	-0. 08009200
H	5. 27656600	-2. 13187700	-0. 55016700
H	1. 89781600	0. 22573700	5. 67754400
H	0. 99417900	-0. 74829200	4. 52491100
H	2. 37595300	-1. 44630000	5. 38507700
H	4. 50606200	1. 59291100	5. 15348600
H	4. 92494500	-0. 10079200	5. 41442200
H	5. 65957100	0. 78088600	4. 08182100
H	1. 14710300	-2. 38861900	3. 12999900
H	1. 11922400	-5. 14077000	-0. 16643300
H	0. 09716200	-4. 23298400	1. 88368600
H	5. 27220300	2. 37525400	2. 71682700
H	4. 96902900	4. 88702700	-0. 73235100
H	6. 27407400	3. 97643100	1. 13593800
H	5. 35708900	-4. 55322200	-0. 63210100

H	6.32029800	-5.52672800	-2.68525100
H	4.88448600	-5.92412400	-4.67555600
H	1.50408100	-4.34727600	-2.54102100
H	2.46852200	-5.34069200	-4.58850100
H	1.22112100	2.92453400	-2.09367100
H	-0.04811600	4.28855100	-3.69982600
H	0.37876900	6.73204000	-3.87689700
H	3.33432600	6.42676500	-0.77953600
H	2.08396000	7.78693400	-2.40225100
H	-0.80008200	0.81148500	1.50821200
H	0.03908800	-0.21539700	2.66989900
H	-0.40331700	1.43287000	3.11458000
H	6.76855600	-0.53022600	0.64748100
H	6.09061200	0.62713400	1.78836200
H	6.71329400	-0.92012700	2.36821700
H	3.38473600	1.46367200	-2.51767000
H	0.98560500	-1.98083300	-0.51834000
H	-1.38398800	-1.53904900	-0.12079200
H	1.11610100	1.21656900	-3.40730300
H	-1.29601300	1.53819300	-3.11251100
H	3.06180900	-1.57619600	-2.08777800
H	4.64867400	0.19783300	-2.63775200
C	-10.36743100	-0.29467300	0.25783900
H	-10.22861000	-1.30645900	-0.14705200
H	-9.97272800	-0.31875900	1.28061100
C	-11.86033600	0.05858200	0.26753300
H	-12.20582500	0.15196400	-0.77169800
H	-11.99666500	1.05197900	0.72083000
C	-12.76986200	-0.95173800	0.99535600
H	-12.60467700	-1.93808500	0.53538900
C	-12.44276900	-1.06855900	2.49204700
H	-13.11672600	-1.77758000	2.98451800
H	-11.41915300	-1.41410200	2.66695500
H	-12.55916700	-0.09952600	2.99358300
C	-14.24716400	-0.58197400	0.79440800
H	-14.50770400	-0.53340200	-0.26854000
H	-14.90818200	-1.31536200	1.26828000
H	-14.46863700	0.39727300	1.23632400
H	4.20571800	0.84206100	-1.08164800
C	-3.01760500	0.31568900	-1.43846500
H	-3.17510500	1.34182200	-1.07791600
H	-3.44861700	0.30066800	-2.44801400
C	-3.81748700	-0.64993100	-0.54501200
H	-3.66929000	-1.67751100	-0.89987200

H	-3.42970400	-0.60974500	0.48068900
C	-5.29586700	-0.32022400	-0.53654000
C	-6.15342900	-0.83823300	-1.51551700
C	-5.83726100	0.54448400	0.42254500
C	-7.50586700	-0.50005600	-1.53488000
H	-5.76035300	-1.51580000	-2.27066100
C	-7.19038700	0.88137400	0.40196800
H	-5.19475400	0.95886800	1.19692000
C	-8.05065600	0.36631800	-0.57702400
H	-8.15003800	-0.91606600	-2.30584100
H	-7.58567500	1.55512000	1.15849200
H	-9.90369600	0.71120100	-1.60295000
H	-9.67417200	1.70979400	-0.17513700