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Supporting Information

Can low-valent silicon compounds be better transition metal ligands than phosphines and NHC?

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1. Tables

Table S1. Proton affinity of low-valent silicon compounds (RI-B97-D/Def2-TZVP//RI-B97-D/6-31G*)

Compound	E (compound) [Hartree]	E (H^+-complex) [Hartree]	Proton affinity [kJ/mol]	Compound	E (compound) [Hartree]	E (H^+-complex) [Hartree]	Proton affinity [kJ/mol]
1	-2367.33	-2367.76	1133	43	-2868.84	-2869.28	1144
2	-2003.82	-2004.24	1104	44	-791.97	-792.347	989
3	-2036.05	-2036.47	1099	45	-1175.29	-1175.66	971
4	-2944.54	-2944.95	1097	46	-1096.69	-1097.05	959
5	-4236.21	-4236.66	1182	47	-1411.09	-1411.45	967
6	-4118.33	-4118.78	1184	48	-793.171	-793.554	1007
7	-1575.84	-1576.32	1270	49	-832.469	-832.856	1018
8	-987.968	-988.406	1150	50	-950.365	-950.754	1020
9	-2062.4	-2062.86	1218	51	-871.769	-872.158	1023
10	-2533.98	-2534.46	1247	52	-1024.16	-1024.53	964
11	-2133.92	-2134.36	1144	53	-1063.46	-1063.83	972
12	-2369.71	-2370.15	1145	54	-1040.2	-1040.57	952
13	-1449,9	-1450,36	1187	55	-2047.13	-2047.51	996
14	-2898.24	-2898.71	1232	56	-2668.64	-2669.09	1193
15	-3818.82	-3819.33	1352	57	-2904.46	-2904.92	1202
16	-1959.96	-1960.43	1210	58	-2081.2	-2081.61	1079
17	-2193.35	-2193.8	1203	59	-2383.48	-2383.89	1088
18	-1893.85	-1894.29	1154	60	-1751.4	-1751.85	1181
19	-2080.3	-2080.74	1144	61	-1908.61	-1909.06	1187
20	-1069.37	-1069.79	1092	62	-1796.87	-1797.33	1211
21	-1083.96	-1084.34	998	63	-1740.59	-1741.03	1151
22	-984.807	-985.234	1120	64	-1971.55	-1972	1187
23	-1024.12	-1024.56	1151	65	-2219.46	-2219.9	1152
24	-1118.77	-1119.21	1153	66	-2758.76	-2759.2	1149
25	-1217.27	-1217.71	1156	67	-3479.99	-3480.46	1241
26	-1177.97	-1178.41	1148	68	-1527.76	-1528.14	999
27	-1562.59	-1563.03	1151	69	-1911.11	-1911.58	1235
28	-2144.1	-2144.54	1154	70	-2068.32	-2068.79	1236
29	-1444.52	-1444.93	1085	71	-1528.97	-1529.42	1190
30	-3559.75	-3560.16	1075	72	-1584.35	-1584.81	1215
31	-2379.62	-2380.07	1199	73	-1702.25	-1702.71	1222
32	-1968.44	-1968.9	1196	74	-1870.6	-1871.06	1199
33	-3285.32	-3285.77	1182	75	-1604.24	-1604.7	1195
34	-4760.87	-4761.31	1144	76	-2489.89	-2490.32	1135
35	-2043.75	-2044.2	1183	77	-1927.23	-1927.68	1168
36	-2664.3	-2664.74	1158	78	-1988.68	-1989.12	1154
37	-2719.09	-2719.54	1192	79	-2898.54	-2898.97	1149
38	-3618.43	-3618.9	1235	80	-3735.76	-3736.09	888
39	-1969.67	-1970.1	1138	81	-1713.32	-1713.77	1192
40	-2429.38	-2429.81	1125	82	-1159.61	-1160.06	1176
41	-1521.76	-1522.22	1233	83	-1036.03	-1036.42	1031
42	-1642.1	-1642.59	1278	84	-1046.93	-1047.34	1072

Table S2. Barriers and relative barriers of P-H bond rotation in the LSi=P-H units (RI-B97-D/Def2-TZVP//RI-B97-D/6-31G*)

Compound	E(LSi=PH complex) [Hartree]	E(transition state) [Hartree]	Rotation barrier [kJ/mol]	Relative rotation barrier	Compound	E(LSi=PH complex) [Hartree]	E (transition state) [Hartree]	Rotation barrier [kJ/mol]	Relative rotation barrier
1	-2709.33	-2709.31	75.44	0.562	44	-1133.94	-1133.93	24.93	0.186
2	-2345.84	-2345.81	76.34	0.569	45	-1517.26	-1517.25	23.45	0.175
3	-2378.05	-2378.02	74.29	0.553	46	-1438.65	-1438.65	23.35	0.174
4	-3286.52	-3286.5	58.36	0.435	47	-1753.05	-1753.05	21.81	0.162
5	-4578.2	-4578.19	30.20	0.225	48	-1135.15	-1135.13	38.13	0.284
6	-4460.31	-4460.3	22.42	0.167	49	-1174.45	-1174.44	36.42	0.271
7	-1917.84	-1917.84	15.26	0.114	50	-1292.35	-1292.33	40.13	0.299
8	-1329.96	-1329.95	21.52	0.160	51	-1213.75	-1213.73	39.40	0.293
9	-2404.39	-2404.38	11.80	0.088	52	-1366.13	-1366.12	23.36	0.174
10	-2875.97	-2875.97	4.12	0.031	53	-1405.43	-1405.43	21.73	0.162
11	-2475.91	-2475.9	15.45	0.115	54	-1382.18	-1382.17	25.79	0.192
12	-2711.7	-2711.69	21.47	0.160	55	-2389.1	-2389.09	24.91	0.186
13	-1792,3	-1792,3	16.36	0.122	56	-3010.63	-3010.62	30.29	0.226
14	-3240.23	-3240.22	15.07	0.112	57	-3246.46	-3246.44	39.56	0.295
15	-4160.8	-4160.8	0.00	0.000	58	-2423.21	-2423.18	79.97	0.596
16	-2301.93	-2301.92	28.15	0.210	59	-2725.49	-2725.46	78.76	0.586
17	-2535.31	-2535.3	28.15	0.210	60	-2093.38	-2093.38	7.96	0.059
18	-2235.84	-2235.82	34.16	0.254	61	-2250.59	-2250.58	15.58	0.116
19	-2422.29	-2422.26	61.44	0.457	62	-2138.86	-2138.85	15.09	0.112
20	-1411.35	-1411.32	57.93	0.431	63	-2082.58	-2082.57	23.15	0.172
21	-1425.94	-1425.93	37.60	0.280	64	-2313.54	-2313.53	25.13	0.187
22	-1326.8	-1326.79	26.65	0.198	65	-2561.45	-2561.44	13.74	0.102
23	-1366.12	-1366.11	26.18	0.195	66	-3100.74	-3100.74	4.11	0.031
24	-1460.76	-1460.76	9.17	0.068	67	-3821.96	-3821.96	11.03	0.082
25	-1559.27	-1559.26	13.24	0.099	68	-1869.75	-1869.73	52.85	0.394
26	-1519.96	-1519.96	11.29	0.084	69	-2253.11	-2253.1	14.87	0.111
27	-1904.58	-1904.57	23.25	0.173	70	-2410.31	Optimization failed	0.00	0.000
28	-2486.09	-2486.09	13.94	0.104	71	-1870.97	-1870.95	32.42	0.241
29	-1786.5	-1786.49	13.84	0.103	72	-1926.35	-1926.34	20.16	0.150
30	-3901.73	-3901.73	14.08	0.105	73	-2044.25	-2044.24	24.85	0.185
31	-2721.61	-2721.6	31.24	0.233	74	-2212.61	-2212.6	19.89	0.148
32	-2310.44	-2310.43	24.13	0.180	75	-1946.24	-1946.23	21.50	0.160
33	-3627.31	-3627.3	32.76	0.244	76	-2831.88	-2831.87	23.06	0.172
34	-5102.87	-5102.86	28.59	0.213	77	-2269.22	-2269.21	22.58	0.168
35	-2385.75	-2385.74	15.90	0.118	78	-2330.66	-2330.65	23.63	0.176
36	-3006.29	-3006.29	16.70	0.124	79	-3240.52	-3240.52	17.81	0.133
37	-3061.08	-3061.07	22.16	0.165	80	-4077.73	-4077.71	56.66	0.422
38	-3960.42	-3960.42	12.66	0.094	81	-2055.29	-2055.28	16.73	0.125
39	-2311.66	-2311.65	26.53	0.198	82	-1501.61	-1501.58	67.66	0.181
40	-2771.37	-2771.36	25.98	0.193	83	-1377.98	-1377.98	0.00	0.000
41	-1863.76	-1863.74	29.37	0.219	84	-1388.9	-1388.89	0.00	0.000
42	-1984.09	-1984.08	13.11	0.098	$H_2Si=PH$	-632.627	-632.576	134.29	1.00
43	-3210.82	-3210.81	24.75	0.184	H2C=PH	-381.22296	-381.0806	373.8	1.00

The P-H rotational barrier method for measuring π-acceptor properties:

When connecting a =P-H unit to the silicon center, a formally double bond is formed whose bond energy is a function of π-acceptor properties of the studied compounds. In our recent study,[18] we quantified this bond strength with the capability of hydrogen rotation in the additional molecule part. High activation energy characterizes strong double bond character, and therefore, strong π-acceptor properties while low rotational barriers indicate the absence of π-donation to the divalent silicon, which can be traced back to low or high occupancy of the 'vacant' silicon p-orbital, respectively. Direct comparison of π-acceptor properties of the silicon and carbene compounds is misleading because of the different absolute strength of Si=P and C=P bonds. Therefore, first we compared the rotational barrier result of **82** and silicon compounds with that of CH_2=PH and SiH_2=PH, respectively, creating a relative value that measures the relative emptiness of 'vacant' p-orbital which makes possible comparison between different type of compounds. In case of phosphines the comparison is simple because they have no π-acceptor ability. In case of 14 and 69, we could not find the very low (< 5 kJ/mol) P-H rotational barrier, therefore, we estimated them as 0.0 in Figure 2 and in Table S2.

We note that we also tried to measure π-acceptor properties with singlet-triplet gap calcualtions and we did find correlation between π-acceptor properties, P-H rotational barrier, and singlet-triplet gap for silylenes but only for silylenes and not for all low-valent silicon compounds. The reason is that for donor stabilized low-valent silylenes the empty p-orbital of the silicon centre is more or less occupied therefore the LUMO orbital, which is needed for the triplet state, is not related to the silicon centre, it is usually related to the π-system of an phenyl ring of the bulky ligand, which gives artifact results for these compounds. Therefore, we chose P-H rotational barrier as a general tool for measuring π-acceptor properties all low-valent silicon compounds.

Table S3. Charge of the Pd atom in Pd complexes (RI-B97-D/6-31G*)

Compound	Pd charge	Compound	Pd charge
1	-0.32	43	-0.30
2	-0.31	44	-0.26
3	-0.31	45	-0.22
4	-0.21	46	-0.22
5	-0.24	47	-0.20
6	-0.25	48	-0.28
7	-0.60	49	-0.28
8	-0.42	50	-0.27
9	-0.32	51	-0.28
10	-0.13	52	-0.24
11	-0.28	53	-0.24
12	-0.28	54	-0.22
13	-0.36	55	-0.24
14	-0.41	56	-0.08
15	-0.07	57	-0.31
16	-0.21	58	-0.29

17	-0.04	59	-0.27
18	-0.37	60	-0.33
19	-0.27	61	-0.31
20	-0.27	62	-0.41
21	-0.29	63	-0.34
22	-0.37	64	-0.34
23	-0.40	65	-0.31
24	-0.39	66	-0.30
25	-0.43	67	-0.45
26	-0.42	68	-0.21
27	-0.37	69	-0.41
28	-0.35	70	-0.41
29	-0.32	71	-0.39
30	-0.29	72	-0.43
31	-0.42	73	-0.43
32	-0.41	74	-0.39
33	-0.29	75	-0.44
34	-0.37	76	-0.32
35	-0.43	77	-0.37
36	-0.50	78	-0.34
37	-0.33	79	-0.34
38	-0.44	80	-0.11
39	-0.32	81	-0.38
40	-0.29	82	-0.21
41	-0.45	83	-0.20
42	-0.49	84	-0.26

Table S4. Buried volume of the palladium atom in palladium complexes (RI-B97-D/6-31G* geometry)

Compound	Coverage	Compound	Coverage
1	0.648	43	0.451
2	0.476	44	0.372
3	0.433	45	0.356
4	0.662	46	0.336
5	0.641	47	0.426
6	0.633	48	0.382
7	0.524	49	0.385
8	0.427	50	0.384
9	0.534	51	0.387
10	0.683	52	0.379
11	0.498	53	0.376
12	0.565	54	0.380
13	0.578	55	0.374
14	0.747	56	0.619
15	0.749	57	0.623
16	0.779	58	0.467

17	0.811	59	0.491
18	0.651	60	0.405
19	0.656	61	0.431
20	0.559	62	0.588
21	0.346	63	0.494
22	0.371	64	0.520
23	0.375	65	0.555
24	0.391	66	0.500
25	0.416	67	0.853
26	0.386	68	0.511
27	0.440	69	0.633
28	0.474	70	0.662
29	0.365	71	0.529
30	0.357	72	0.525
31	0.592	73	0.556
32	0.471	74	0.611
33	0.752	75	0.525
34	0.412	76	0.582
35	0.415	77	0.527
36	0.689	78	0.527
37	0.458	79	0.631
38	0.676	80	0.513
39	0.413	81	0.674
40	0.411	82	0.543
41	0.443	83	0.322
42	0.534	84	0.374

2. Optimized geometries (RI-B97-D/6-31G*)

2.1. Basic structures

1
C 1.863815 -3.309170 -0.669230
C 1.012053 -2.981004 0.412205
C 1.413834 -3.160436 1.761875
C 2.696965 -3.683090 2.002688
C 3.548492 -4.027885 0.945559
C 3.131380 -3.845222 -0.377584
N -0.297300 -2.459101 0.147122
C -1.394928 -3.300880 -0.071711
C -2.522372 -2.539418 -0.149834
N -2.178411 -1.184861 0.007797
C -3.187344 -0.171120 0.016039
C -3.431092 0.554981 1.210718
C -4.398470 1.576790 1.185157
C -5.133482 1.854313 0.028286
C -4.909234 1.100042 -1.128442
C -3.935683 0.086631 -1.163632
C -2.745986 0.227206 2.536636

C -3.761501 -0.392670 3.525110
C -3.732758 -0.700601 -2.458824
C -3.529747 0.219990 -3.683097
C 0.460812 -2.864486 2.918939
C -0.320919 -4.145512 3.297146
C 1.409168 -3.135049 -2.115169
C 2.499624 -2.511318 -3.012246
B -0.735400 -1.070712 0.208686
Si 0.599928 0.296960 1.010934
N 0.918321 1.491396 -0.245040
C 2.013583 2.395642 0.060962
C 3.325491 2.045302 -0.359134
C 4.384756 2.920617 -0.064967
C 4.164150 4.124154 0.615542
C 2.868133 4.458343 1.019189
C 1.777208 3.609367 0.753446
C 3.608463 0.719069 -1.063569
C 4.140813 -0.317399 -0.047169
C 0.390436 4.014218 1.245313
C -0.049469 5.373827 0.657460
Si 0.108593 1.814010 -1.826459
C -1.552350 2.676164 -1.511257
C 1.213911 2.984152 -2.838808
C -0.081300 0.197211 -2.802503
C 4.581248 0.854451 -2.254612
C 0.351198 4.050758 2.790202
C -2.065414 1.465108 3.157384
C -4.929121 -1.649889 -2.707133
C 1.161772 -2.263996 4.154254
C 0.941174 -4.488918 -2.698851
H 0.736388 3.201606 -3.810690
H 1.380571 3.940512 -2.318291
H 2.202505 2.541145 -3.037029
H -0.431883 0.410402 -3.827057
H 0.893111 -0.309319 -2.880399
H -0.789692 -0.502905 -2.338476
H -2.132267 2.774110 -2.444219
H -2.177157 2.129856 -0.790431
H -1.385809 3.690726 -1.115415
H 5.397344 2.653662 -0.373182
H 4.999011 4.794402 0.832469
H 2.691334 5.392033 1.557861
H 2.656601 0.333157 -1.455200
H 4.330575 -1.284767 -0.538041
H 5.080102 0.043602 0.403935
H 3.414539 -0.482679 0.765344
H 4.656085 -0.109155 -2.784273
H 4.241237 1.621493 -2.968654
H 5.594750 1.126749 -1.918695
H -0.329953 3.257183 0.907887
H -1.080056 5.609182 0.971275
H 0.607817 6.185614 1.009378
H -0.012693 5.362508 -0.443515
H -0.661030 4.308132 3.143830
H 0.631597 3.071722 3.207978
H 1.055107 4.805539 3.177458

H -1.276145 -4.376998 -0.154957
H -3.553301 -2.841373 -0.302509
H -4.587234 2.146296 2.097195
H -5.882719 2.649036 0.029843
H -5.488115 1.307991 -2.030123
H -1.968596 -0.526893 2.358866
H -3.259631 -0.651758 4.472333
H -4.573267 0.319757 3.746711
H -4.210911 -1.306126 3.104579
H -1.493469 1.176726 4.053295
H -1.370890 1.937789 2.447042
H -2.810345 2.221871 3.454261
H -2.830366 -1.318054 -2.357203
H -4.768108 -2.236381 -3.626882
H -5.069786 -2.348863 -1.867989
H -5.860209 -1.071347 -2.824115
H -3.319750 -0.390187 -4.576767
H -4.432026 0.818166 -3.888905
H -2.688492 0.907057 -3.522368
H 3.031091 -3.826766 3.031048
H 4.539931 -4.436000 1.154669
H 3.799480 -4.113148 -1.198081
H 0.546565 -2.455770 -2.116999
H 0.598781 -4.360352 -3.739412
H 1.767920 -5.218779 -2.692686
H 0.110254 -4.904418 -2.108049
H 2.085948 -2.304987 -4.012570
H 2.873239 -1.568408 -2.586733
H 3.356576 -3.192701 -3.139308
H -0.274010 -2.124810 2.571846
H -1.028205 -3.932101 4.116144
H -0.890749 -4.524784 2.435067
H 0.373232 -4.933966 3.633314
H 0.403243 -1.977835 4.900938
H 1.838436 -2.991656 4.632091
H 1.739072 -1.368442 3.879299

2

C -2.141495 -3.000407 -0.566237
Si -2.821085 -1.215098 -0.515898
C -3.334738 -0.743300 -2.288798
C -1.469898 -0.031265 0.147430
Si -2.153409 1.700208 0.635195
C -2.937293 1.572056 2.369289
Si 0.030349 0.128148 -1.061451
C 1.504802 0.144901 0.197562
Si 2.980698 1.175462 -0.465909
C 3.925839 0.174294 -1.786353
H -1.105667 -0.423613 1.117242
H 1.151203 0.588316 1.151005
Si 1.987966 -1.654441 0.672527
C 0.744869 -2.328259 1.954626
C -0.742168 2.985192 0.730063
C -3.440279 2.350850 -0.609784
C -4.369140 -1.210871 0.603146
C 1.977709 -2.777035 -0.871037

C 3.717609 -1.767185 1.473313
C 2.386170 2.796003 -1.284545
C 4.148294 1.667790 0.961639
H -4.026668 -1.500499 -2.697833
H -3.843546 0.232213 -2.330721
H -2.458686 -0.691053 -2.956721
H -5.097313 -1.965201 0.256414
H -4.115243 -1.449651 1.649889
H -4.876842 -0.232117 0.598236
H -2.893013 -3.686665 -0.994748
H -1.235635 -3.070405 -1.192796
H -1.881206 -3.381813 0.435441
H -3.291088 2.560475 2.712036
H -3.794641 0.880981 2.382828
H -2.201942 1.208079 3.107788
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20

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21

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31

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41

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42

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43

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66

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2.2. H^+-complexes

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H -3.907216 -2.827370 3.377362
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7-H$^+$
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8-H$^+$
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12-H$^+$
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13-H$^+$
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C 2.456006 0.013741 0.171540
C 3.183604 1.208335 -0.013309
C 4.512284 1.074863 -0.454417
C 5.068748 -0.186618 -0.698999
C 4.308296 -1.348334 -0.510389
C 2.974283 -1.279331 -0.069900
C 2.592435 2.591109 0.250495
C 3.289545 3.255198 1.461489
C 2.170300 -2.553176 0.189582
C 2.595062 -3.176882 1.541337
Si 0.019117 -0.045325 -2.081648
C -2.226503 -2.532626 0.279570
C -2.163611 -3.434658 -0.974178
C -2.553883 2.623054 0.169420
C -2.552767 3.430378 -1.150038
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C -2.841858 -3.296192 1.476046
C -3.292997 3.396725 1.286328
C 2.303791 -3.582155 -0.954284
C 2.684394 3.493600 -1.001812
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H 1.416835 0.227020 2.761170
H -4.802668 -2.286859 -0.589493
H -6.115364 -0.217405 -1.009958

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H 5.111500 1.973088 -0.608029
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H -2.068615 4.406596 -0.991540
H -2.014192 2.895140 -1.948159
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H -1.191171 -2.274838 0.553082
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H -2.851861 -2.673369 2.384486
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H -3.170545 -3.766627 -1.270234
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H 3.196468 2.634645 2.367187
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H 1.140451 0.803452 -2.545029

14-H$^+$
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C 4.077502 -0.179976 -0.141325
C 4.015569 0.899158 0.776723
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C 5.428995 2.153305 -0.774335
C 5.457119 1.070799 -1.659576
N 3.360880 -1.389876 0.199529
C 1.997906 -1.503226 0.089028
N 1.701697 -2.700599 0.690350
C 2.861683 -3.317482 1.151769
C 3.904563 -2.489887 0.848124
C 0.372880 -3.130055 1.070367
C -0.023847 -2.904883 2.407685
C -1.308908 -3.345438 2.777230
C -2.157793 -3.951570 1.846764
C -1.737181 -4.144710 0.523655
C -0.455494 -3.749374 0.105656
C 0.876365 -2.236394 3.447556
C 0.168129 -1.064780 4.163733
C 0.044991 -3.994298 -1.316715

C 1.011370 -5.204012 -1.349951
Si 1.035570 -0.234648 -1.041501
Si -0.744740 0.000809 0.232129
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C -4.953942 -2.691404 -1.154474
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C -4.364728 -0.734031 0.184554
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C -0.782208 3.925623 1.304174
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15-H$^+$

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H 2.569220 2.020868 -2.863584
H 0.062367 -0.638695 -0.413527

17-H$^+$
C 2.435176 -1.404572 2.190450
C 2.583861 -1.282736 0.783456
C 2.578699 -2.419392 -0.070130
C 2.512739 -3.688701 0.532938
C 2.432333 -3.835737 1.920769
C 2.374016 -2.700447 2.734062
N 2.731127 0.039469 0.207354
C 1.697633 0.842277 -0.145630
C 2.260443 2.058983 -0.893320
C 3.732112 2.096379 -0.407152
C 4.102756 0.657181 0.008495
C 2.142576 1.746199 -2.426722
C 2.724837 2.871897 -3.305742
C 2.070870 4.229487 -2.979731
C 2.159832 4.541677 -1.472674
C 1.543138 3.397728 -0.640147
Si -0.000019 0.169680 -0.004614
C -1.696762 0.843069 0.147402
N -2.731389 0.041710 -0.204800
C -4.102297 0.660064 -0.001434
C -3.729687 2.098307 0.415636
C -2.256676 2.059311 0.897683
C -2.134956 1.744023 2.430266
C -2.714447 2.868626 3.312490
C -2.061324 4.226641 2.986535
C -2.154144 4.540999 1.480133
C -1.539349 3.398103 0.644700
C -2.585937 -1.278726 -0.785816
C -2.579455 -2.418627 0.063445
C -2.515560 -3.685593 -0.544797
C -2.437670 -3.827246 -1.933307
C -2.380365 -2.688850 -2.742328

C -2.440260 -1.395052 -2.193689
C -2.551803 -2.351844 1.591835
C -3.725746 -3.125351 2.239344
C -2.263489 -0.202448 -3.133461
C -3.310853 -0.185077 -4.270991
C -4.901356 0.633889 -1.315949
C -4.912256 -0.093927 1.067341
C 4.897716 0.628112 1.325538
C 4.915643 -0.095068 -1.059297
C 2.554678 -2.346516 -1.598231
C 3.727122 -3.121779 -2.246143
C 2.255657 -0.215494 3.134030
C 3.300154 -0.201871 4.274327
C 1.225402 -2.915344 -2.156862
C 0.830774 -0.235925 3.740400
C -0.840132 -0.219950 -3.743502
C -1.224093 -2.928912 2.145828
H -3.801767 2.768520 -0.455744
H -4.412767 2.480284 1.183987
H -2.276100 -2.797304 -3.822650
H -2.397276 -4.821391 -2.382112
H -2.515593 -4.572575 0.090007
H -2.362854 0.725139 -2.552395
H -3.172324 0.714080 -4.892227
H -3.190192 -1.064407 -4.922592
H -4.339015 -0.188495 -3.883210
H -0.682724 0.679663 -4.360755
H -0.072148 -0.248905 -2.956207
H -0.705181 -1.104446 -4.385755
H -2.608190 -1.298695 1.897759
H -1.223024 -2.857304 3.245174
H -1.121241 -3.991258 1.874423
H -0.345067 -2.394793 1.767005
H -3.703012 -2.986653 3.331884
H -4.706612 -2.800255 1.867844
H -3.629826 -4.203714 2.037781
H 3.802071 2.765026 0.465615
H 4.417541 2.479296 -1.172917
H 2.267518 -2.813027 3.813741
H 2.390611 -4.831570 2.365689
H 2.513277 -4.573119 -0.105441
H 2.355904 0.714296 2.556662
H 0.671490 0.661494 4.360375
H 0.064714 -0.262406 2.951182
H 0.694607 -1.122657 4.379312
H 3.158500 0.693903 4.899741
H 3.179163 -1.084725 4.921058
H 4.329338 -0.201546 3.889186
H 2.615952 -1.292536 -1.899946
H 1.228681 -2.844078 -3.256245
H 1.114453 -3.976841 -1.885242
H 0.348995 -2.374769 -1.781089
H 3.707896 -2.977863 -3.338076
H 4.708177 -2.802081 -1.870274
H 3.626722 -4.200756 -2.050073
H 0.491667 3.285619 -0.939683

H 1.572662 3.640841 0.434006
H 1.631817 5.480994 -1.244795
H 3.214092 4.687537 -1.181158
H 1.006228 4.194032 -3.273841
H 2.543606 5.032081 -3.567142
H 2.563091 2.611761 -4.364195
H 3.816074 2.942180 -3.162479
H 1.072599 1.631003 -2.658310
H 2.622686 0.784290 -2.657477
H -0.487509 3.285404 0.942450
H -1.570512 3.642539 -0.429098
H -1.626516 5.480561 1.252340
H -3.209064 4.687465 1.191401
H -0.995891 4.190757 3.277727
H -2.532466 5.028383 3.576383
H -2.549733 2.607074 4.370131
H -3.806064 2.939184 3.172381
H -1.064446 1.627829 2.658825
H -2.615082 0.781928 2.660437
H -5.042458 -0.396225 -1.672375
H -5.891381 1.075824 -1.127511
H -4.402585 1.220235 -2.097606
H -5.106278 -1.121556 0.734910
H -4.409377 -0.121459 2.041394
H -5.880069 0.414956 1.190961
H 5.885469 0.411503 -1.176327
H 5.104968 -1.124608 -0.730111
H 4.417421 -0.117060 -2.035873
H 5.888150 1.071066 1.141714
H 4.395865 1.212065 2.107012
H 5.038128 -0.402862 1.679805
H -0.000987 -1.287240 0.007063

18-H$^+$

C	-3.102232	2.223179	-1.495225
C	-1.655599	2.276923	-1.435237
C	-1.319508	2.880526	-0.095259
C	-2.582855	3.139808	0.551766
C	-3.644756	2.734048	-0.295048
Si	-1.270379	0.873879	-0.067949
N	0.251755	0.249939	-0.069647
C	0.865002	-0.882132	0.182162
N	2.228936	-1.047089	0.243989
C	2.534442	-2.382124	0.503636
C	1.355550	-3.063255	0.594387
N	0.330310	-2.135971	0.406618
C	3.161870	0.044373	0.112456
C	3.773730	0.255187	-1.144741
C	4.633018	1.361573	-1.258671
C	4.861161	2.214441	-0.169071
C	4.242284	1.971138	1.062051
C	3.378085	0.873781	1.232773
C	3.465355	-0.648380	-2.339174
C	2.205192	-0.133984	-3.078121
C	2.718341	0.622040	2.586969
C	3.775097	0.453914	3.702580

C	-1.086696	-2.370210	0.366182
C	-1.800580	-2.393681	1.587260
C	-3.200940	-2.494279	1.507866
C	-3.851490	-2.562262	0.267502
C	-3.113407	-2.551419	-0.921758
C	-1.709262	-2.455156	-0.900355
C	-1.082937	-2.256731	2.930256
C	-1.773147	-3.031804	4.072257
C	-0.915186	-2.485151	-2.204466
C	-1.402460	-1.412880	-3.202173
C	-0.934720	-0.761824	3.306567
C	-0.985082	-3.895638	-2.836421
C	1.727881	1.756853	2.934526
C	4.645506	-0.792618	-3.322610
C	-3.880607	1.629778	-2.633448
C	-5.106881	2.765006	0.065247
C	-2.732464	3.673363	1.947135
C	-0.008134	3.595589	0.185155
C	-0.727473	2.367536	-2.635056
H	3.562073	-2.710006	0.602001
H	1.140850	-4.110071	0.771699
H	4.432592	2.632850	1.908439
H	5.531410	3.068760	-0.281269
H	5.129951	1.558715	-2.208303
H	3.233055	-1.654986	-1.956593
H	4.400122	-1.551216	-4.081683
H	4.844710	0.152407	-3.852302
H	5.567010	-1.099776	-2.804452
H	1.948841	-0.810422	-3.910094
H	1.344805	-0.064086	-2.397698
H	2.396103	0.868458	-3.495415
H	2.142317	-0.314135	2.533621
H	1.253914	1.561567	3.909779
H	2.250597	2.725115	2.993067
H	0.944737	1.830704	2.166741
H	3.278488	0.231353	4.660435
H	4.472062	-0.365899	3.468966
H	4.362817	1.376331	3.830803
H	-3.626871	-2.629920	-1.881253
H	-4.939878	-2.638509	0.230828
H	-3.788859	-2.521439	2.425136
H	-0.067980	-2.668636	2.818568
H	-1.138391	-3.001132	4.970813
H	-2.742400	-2.580103	4.336837
H	-1.944102	-4.084391	3.799104
H	-0.402870	-0.663032	4.266223
H	-0.367863	-0.209572	2.543443
H	-1.927818	-0.295022	3.412003
H	0.140189	-2.271933	-1.983752
H	-0.781915	-1.435478	-4.111257
H	-2.448537	-1.588700	-3.498894
H	-1.329206	-0.407590	-2.760954
H	-0.388955	-3.924980	-3.762240
H	-0.595940	-4.658552	-2.144266
H	-2.025148	-4.158679	-3.086445
H	-2.498017	0.304252	0.521874

H	-5.664931	1.971648	-0.454827
H	-5.254489	2.638299	1.148748
H	-5.565813	3.728227	-0.217147
H	-3.504309	3.123216	2.509208
H	-1.785803	3.619614	2.503380
H	-3.048734	4.730952	1.920735
H	0.030748	4.533979	-0.392650
H	0.081990	3.842685	1.251764
H	0.854416	2.974456	-0.094306
H	-0.707742	3.405405	-3.006884
H	0.296254	2.073815	-2.367417
H	-1.070096	1.715974	-3.451001
H	-4.739298	1.041667	-2.272792
H	-4.284267	2.428964	-3.279940
H	-3.248100	0.983239	-3.257214

19-H$^+$

C	1.150584	-2.866651	-1.113279
C	0.888874	-1.513103	-1.567743
C	-0.608576	-1.409008	-1.704375
C	-1.132381	-2.706450	-1.320760
C	-0.067634	-3.569639	-0.968817
Si	0.024193	-0.680556	0.029874
C	0.033369	1.087263	0.642828
C	-1.216694	1.620524	1.052900
C	-1.240471	2.789849	1.832001
C	-0.047064	3.437915	2.179977
C	1.184088	2.928338	1.745362
C	1.243113	1.750989	0.978496
C	-2.494812	0.932250	0.671133
C	-3.239720	1.397464	-0.453020
C	-4.445630	0.754658	-0.768496
C	-4.946775	-0.315576	-0.005022
C	-4.204114	-0.746938	1.102758
C	-2.981378	-0.145728	1.461526
C	-2.791525	2.625357	-1.253184
C	-3.153336	2.578742	-2.755202
C	-2.273457	-0.582421	2.746748
C	-2.276901	-2.111764	2.961626
C	-6.270868	-0.975557	-0.369244
C	-7.436594	0.037417	-0.283963
C	2.558407	1.190712	0.537126
C	3.289524	1.833161	-0.501739
C	4.488134	1.240469	-0.934621
C	4.987264	0.055563	-0.368049
C	4.273343	-0.528190	0.690634
C	3.069674	0.020489	1.168448
C	2.790617	3.143314	-1.130041
C	1.653395	2.904480	-2.152831
C	6.286061	-0.565466	-0.868107
C	6.040453	-1.976242	-1.452046
C	2.451513	-0.521893	2.464571
C	2.506973	-2.057289	2.606328
C	3.904856	3.986992	-1.783515
C	7.350658	-0.619655	0.252123
C	3.153550	0.157147	3.666597

C	-2.915881	0.135942	3.957890
C	-6.211442	-1.616890	-1.775362
C	-3.412539	3.906532	-0.639888
C	-2.592556	-3.026180	-1.257759
C	-0.231605	-4.971417	-0.440979
C	2.530294	-3.382116	-0.848438
C	1.880031	-0.708722	-2.386695
C	-1.314321	-0.457137	-2.653737
H	-2.199307	3.180659	2.172998
H	-0.076335	4.338491	2.795794
H	2.114721	3.431304	2.012955
H	5.062002	1.710152	-1.734372
H	4.688100	-1.409675	1.181392
H	-4.598331	-1.562107	1.712642
H	-5.025220	1.103767	-1.623604
H	-1.223266	-0.255823	2.699244
H	-1.647505	-2.365582	3.828822
H	-3.291116	-2.487286	3.169020
H	-1.888377	-2.645955	2.079517
H	-2.405194	-0.154117	4.890259
H	-2.847714	1.228881	3.846469
H	-3.979749	-0.137291	4.043005
H	-6.459713	-1.777337	0.364744
H	-7.175573	-2.090459	-2.018584
H	-6.004326	-0.853362	-2.542869
H	-5.423365	-2.384445	-1.830418
H	-8.391431	-0.462489	-0.510927
H	-7.502702	0.482226	0.720993
H	-7.296455	0.852572	-1.012272
H	-1.695960	2.709910	-1.169438
H	-3.084406	4.793755	-1.205087
H	-4.511796	3.850108	-0.690064
H	-3.122056	4.038857	0.410843
H	-2.687415	3.435663	-3.265746
H	-2.811199	1.656198	-3.243942
H	-4.241236	2.663442	-2.904548
H	1.392739	-0.225177	2.510466
H	1.979757	-2.359102	3.524766
H	2.031947	-2.563343	1.752716
H	3.543533	-2.419075	2.689203
H	2.712790	-0.191374	4.614499
H	4.227426	-0.088613	3.667960
H	3.049959	1.251630	3.612148
H	2.362264	3.752544	-0.320677
H	1.253962	3.870274	-2.501593
H	2.036799	2.359794	-3.030936
H	0.825404	2.330342	-1.708440
H	3.497797	4.968319	-2.070928
H	4.748008	4.146019	-1.093818
H	4.290358	3.507619	-2.697883
H	6.673759	0.075418	-1.677755
H	6.981044	-2.398254	-1.839580
H	5.658707	-2.656622	-0.673075
H	5.307428	-1.945336	-2.274331
H	8.292960	-1.034943	-0.138694
H	7.550535	0.384131	0.657640

H	7.012145	-1.263610	1.080176
H	-0.117204	-1.698147	1.080866
H	2.005881	-1.183040	-3.374563
H	1.525776	0.315689	-2.539819
H	2.854487	-0.658532	-1.885840
H	-1.241214	-0.837879	-3.686081
H	-2.372264	-0.358942	-2.378142
H	-0.865576	0.545395	-2.627492
H	-2.766328	-4.071402	-0.968508
H	-3.101066	-2.369537	-0.533859
H	-3.069016	-2.843667	-2.235788
H	0.726894	-5.507796	-0.423138
H	-0.637708	-4.965771	0.585054
H	-0.930208	-5.548829	-1.066148
H	2.528227	-4.257364	-0.184644
H	3.005408	-3.677096	-1.801797
H	3.159783	-2.595220	-0.409992

20-H$^+$

C	2.322825	-1.222016	-0.193625
C	1.677225	-0.555757	0.943961
C	1.840380	0.919474	0.694506
C	2.518294	1.048595	-0.547717
C	2.812242	-0.250456	-1.076676
Si	-0.000194	-0.000199	0.084505
C	-1.839625	-0.918043	0.695882
C	-1.677653	0.557749	0.942999
C	-2.323490	1.221680	-0.195625
C	-2.812292	0.248413	-1.077271
C	-2.517493	-1.049530	-0.546328
C	-1.663803	1.159178	2.343439
C	-2.372948	2.714716	-0.355002
C	-3.480512	0.477272	-2.405801
C	-2.845484	-2.339897	-1.238079
C	-1.728484	-1.988423	1.763841
C	1.728548	1.991777	1.760409
C	2.847455	2.337604	-1.241471
C	3.480349	-0.481686	-2.404849
C	2.371552	-2.715352	-0.350536
C	1.663381	-1.154906	2.345412
H	0.000187	-0.000604	-1.385525
H	-3.492155	1.541017	-2.679914
H	-2.970102	-0.081715	-3.207948
H	-4.525264	0.123696	-2.384208
H	-2.508123	-2.326711	-2.287818
H	-2.394674	-3.204163	-0.731185
H	-3.939001	-2.491280	-1.260930
H	-1.444374	-2.959875	1.333102
H	-0.987853	-1.723709	2.529724
H	-2.700783	-2.114064	2.269086
H	-2.512152	3.011752	-1.404053
H	-3.212402	3.136600	0.225974
H	-1.451779	3.187171	0.021000
H	-1.330839	2.205956	2.321901
H	-2.683110	1.127857	2.761114
H	-1.005226	0.598449	3.022292

H	2.682896	-1.123927	2.762592
H	1.005645	-0.592404	3.023618
H	1.329364	-2.201379	2.325736
H	2.509755	-3.014184	-1.399216
H	3.211312	-3.136643	0.230430
H	1.450500	-3.186828	0.026968
H	3.493701	-1.546129	-2.676151
H	2.968675	0.074309	-3.208295
H	4.524478	-0.126215	-2.384582
H	2.509682	2.323225	-2.291065
H	2.397741	3.203099	-0.735702
H	3.941121	2.487780	-1.264956
H	2.700311	2.117865	2.266600
H	1.445467	2.962610	1.327589
H	0.986914	1.728872	2.525943

21-H$^+$

C 0.084302 2.013015 1.585405
Si 0.000049 1.018803 -0.000107
C -0.083888 2.013021 -1.585628
Si -0.000110 -1.482948 -0.000277
N -1.231703 -0.342213 0.046810
C -2.724343 -0.351479 0.012884
C -3.215940 -1.768073 0.361181
N 1.231645 -0.342419 -0.047239
C 2.724265 -0.351588 -0.012697
C 3.215994 -1.768196 -0.360832
C 3.239921 0.665855 -1.050198
C 3.187741 0.044473 1.405280
C -3.239622 0.665969 1.050586
C -3.188331 0.044575 -1.404934
H 4.287150 0.046677 1.449972
H 2.829483 1.051507 1.666213
H 2.808081 -0.671219 2.151078
H 4.339818 0.660284 -1.055758
H 2.879888 0.413561 -2.058932
H 2.910192 1.686834 -0.797794
H 4.314895 -1.796569 -0.353081
H 2.858810 -2.501904 0.382457
H 2.870491 -2.066006 -1.364397
H -4.287755 0.046989 -1.449194
H -2.829959 1.051517 -1.666068
H -2.809081 -0.671238 -2.150822
H -4.314850 -1.796363 0.354070
H -2.859271 -2.501764 -0.382371
H -2.869911 -2.066035 1.364528
H -4.339514 0.660314 1.056676
H -2.879085 0.413736 2.059155
H -2.910073 1.686952 0.797963
H -0.792630 2.672684 1.686136
H 0.123522 1.353026 2.465601
H 0.982037 2.653260 1.595593
H -0.981865 2.652911 -1.596375
H 0.792840 2.673051 -1.685835
H -0.122288 1.353008 -2.465840
H -0.000257 -2.960188 -0.000881

22-H$^+$
C 0.364677 3.310760 -1.161905
C 0.378070 1.910113 -1.163971
C -0.000492 1.208758 -0.000100
C -0.379760 1.909487 1.163926
C -0.367824 3.310146 1.162139
C -0.001939 4.010445 0.000187
C 0.000188 -0.263210 -0.000164
N -1.081105 -1.079952 0.128952
C -2.548737 -0.817892 -0.073087
C -3.133241 -0.107454 1.164366
N 1.082129 -1.079064 -0.129102
Si 0.001093 -2.518531 0.000193
C 2.549504 -0.815732 0.072975
C 3.133342 -0.104164 -1.164145
C 2.772199 0.018957 1.349624
C 3.199157 -2.205725 0.227036
C -2.772188 0.017170 -1.349345
C -3.197051 -2.208429 -0.227835
H 0.147402 -3.314724 1.235718
H -0.652736 1.359058 2.064430
H -0.644056 3.853362 2.066733
H -0.002510 5.101367 0.000303
H 0.640335 3.854441 -2.066394
H 0.651607 1.360152 -2.064591
H 4.286244 -2.092685 0.340150
H 2.819223 -2.724949 1.122018
H 3.017233 -2.825570 -0.667440
H 3.853932 0.124118 1.519839
H 2.339744 1.023853 1.253776
H 2.331168 -0.482255 2.225658
H 4.227796 -0.055378 -1.062156
H 2.893723 -0.659322 -2.083914
H 2.752300 0.921709 -1.248604
H -4.284247 -2.096361 -0.340898
H -2.816584 -2.726870 -1.123030
H -3.014590 -2.828527 0.666366
H -3.854024 0.121294 -1.519567
H -2.340795 1.022472 -1.253021
H -2.330608 -0.483182 -2.225590
H -4.227739 -0.059618 1.062395
H -2.893117 -0.662822 2.083877
H -2.753119 0.918722 1.249314
H -0.144481 -3.315119 -1.235228

23-H$^+$
C 3.578604 -0.406279 -0.966159
C 2.182319 -0.370357 -1.077718
C 1.403076 -0.018394 0.043536
C 2.021003 0.286605 1.273521
C 3.416684 0.227995 1.380192
C 4.195170 -0.113696 0.261717
C -0.067591 0.016091 -0.064894
N -0.864921 1.116302 -0.001450
C -0.541814 2.569749 -0.196599

C 0.208617 3.122305 1.031902
N -0.894196 -1.045273 -0.246469
Si -2.320651 0.072981 -0.279329
C -3.548858 -0.049250 1.118795
C -0.663351 -2.518917 -0.085171
C 0.047989 -3.076658 -1.334825
C 0.155845 -2.805632 1.189290
C -2.064956 -3.149938 0.039865
C 0.287068 2.759350 -1.482765
C -1.904504 3.278975 -0.330216
H 1.409732 0.544772 2.138609
H 3.894976 0.449866 2.335090
H 5.282132 -0.151212 0.346806
H 4.183114 -0.663045 -1.837025
H 1.697690 -0.587124 -2.029969
H -1.968946 -4.242545 0.104723
H -2.578722 -2.796918 0.947533
H -2.681321 -2.919637 -0.846278
H 0.208586 -3.894560 1.336556
H 1.180273 -2.420063 1.106947
H -0.327600 -2.359679 2.072742
H 0.097234 -4.173398 -1.259702
H -0.505969 -2.814246 -2.249183
H 1.073498 -2.691894 -1.408598
H -1.746675 4.359255 -0.454531
H -2.456340 2.916665 -1.213770
H -2.514942 3.125802 0.574793
H 0.457080 3.833907 -1.646841
H 1.264543 2.264118 -1.401814
H -0.250610 2.356266 -2.355632
H 0.296471 4.214576 0.932272
H -0.343871 2.900370 1.957780
H 1.220535 2.703321 1.103321
H -4.138799 0.879384 1.195915
H -4.254565 -0.878621 0.950365
H -3.034962 -0.214671 2.078533
H -2.891416 0.228677 -1.635425

24-H$^+$
C -4.043370 -0.488202 -0.784516
C -2.659555 -0.444604 -0.998854
C -1.801741 -0.078017 0.058305
C -2.329456 0.228399 1.329042
C -3.713081 0.159758 1.539627
C -4.570153 -0.191216 0.483525
C -0.346055 -0.006425 -0.172494
N 0.489373 -1.040821 -0.427499
C 0.331579 -2.512944 -0.195016
C -0.233853 -2.765819 1.217309
N 0.420784 1.117605 -0.188971
Si 1.872135 0.125854 -0.656027
N 3.175282 0.124963 0.416587
C 4.582810 -0.010753 0.003170
C 0.038815 2.564618 -0.306612
C -1.051582 2.763065 -1.378231
C -0.432215 3.089090 1.064977

C 1.327661 3.302292 -0.725540
C 2.980168 0.096053 1.875356
C -0.579849 -3.132749 -1.273356
C 1.749557 -3.109882 -0.306299
H -1.658693 0.493364 2.146785
H -4.120463 0.381542 2.526915
H -5.647652 -0.234222 0.648698
H -4.708405 -0.755520 -1.606788
H -2.244608 -0.665621 -1.982477
H 1.129451 4.381934 -0.778507
H 2.131676 3.133144 0.008569
H 1.668534 2.970231 -1.719845
H -0.583400 4.177053 1.000507
H -1.384239 2.628059 1.358454
H 0.324695 2.887273 1.838564
H -1.222657 3.841330 -1.514597
H -0.729889 2.339229 -2.342733
H -2.001303 2.299665 -1.080802
H 1.697500 -4.197501 -0.158239
H 2.177409 -2.922182 -1.305019
H 2.417623 -2.685999 0.459366
H -0.571590 -4.227629 -1.162903
H -1.615735 -2.785612 -1.165476
H -0.215284 -2.881637 -2.281267
H -0.272080 -3.850034 1.399300
H 0.414328 -2.308113 1.981415
H -1.250772 -2.363663 1.320036
H 4.994227 -0.976652 0.344661
H 4.672296 0.043861 -1.091644
H 5.180293 0.803642 0.446064
H 3.294310 -0.877261 2.292559
H 3.583523 0.889694 2.347579
H 1.922976 0.267486 2.129467
H 2.311889 0.243968 -2.057436

25-H$^+$
C 5.090947 -0.131089 0.546682
C 4.577882 -0.408704 -0.731519
C 3.195207 -0.380532 -0.955057
C 2.325381 -0.047324 0.103420
C 2.839001 0.241474 1.384323
C 4.221877 0.186453 1.603612
C 0.869532 0.000295 -0.127695
N 0.059157 -1.049320 -0.420042
C 0.236106 -2.519846 -0.169275
C -1.145001 -3.157082 -0.420320
N 0.078796 1.106980 -0.104974
Si -1.334117 0.083336 -0.604756
O -2.523565 -0.100023 0.473866
C -4.007615 0.016460 0.349507
C -4.493653 -1.008434 -0.684105
C 0.438647 2.557378 -0.265449
C -0.898942 3.290519 -0.492189
C 1.102764 3.089010 1.020586
C 1.361578 2.747462 -1.485874
C 1.269959 -3.116974 -1.144369

C 0.662464 -2.742389 1.296006
C -4.539799 -0.301540 1.749882
C -4.343177 1.453314 -0.069900
H 2.157390 0.487451 2.198946
H 4.619227 0.394214 2.597989
H 6.167720 -0.163248 0.719091
H 5.252740 -0.650625 -1.553619
H 2.788729 -0.595651 -1.943580
H -1.074540 -4.243580 -0.271354
H -1.893846 -2.756652 0.279150
H -1.478285 -2.974841 -1.455537
H 0.730508 -3.823011 1.491165
H 1.645861 -2.293726 1.494725
H -0.080028 -2.308802 1.983999
H 1.262737 -4.212302 -1.039588
H 1.014902 -2.865648 -2.185311
H 2.283842 -2.759857 -0.923111
H -0.713277 4.369319 -0.588017
H -1.385679 2.949185 -1.420811
H -1.581141 3.129460 0.357125
H 1.560169 3.820685 -1.624897
H 2.322547 2.234807 -1.342055
H 0.880898 2.363285 -2.399839
H 1.205491 4.181606 0.939841
H 0.482480 2.860598 1.900575
H 2.103875 2.661798 1.160993
H -5.638108 -0.236004 1.746360
H -4.248918 -1.319016 2.050576
H -4.145144 0.415831 2.484313
H -5.435254 1.581672 -0.109693
H -3.934129 2.171502 0.656205
H -3.939359 1.677803 -1.070604
H -5.591357 -0.970150 -0.750081
H -4.087168 -0.788532 -1.684426
H -4.198846 -2.026167 -0.388616
H -1.732486 0.307752 -2.008743

26-H$^+$
C 4.886462 -0.078391 0.619359
C 4.402469 -0.355894 -0.670200
C 3.024207 -0.346079 -0.920635
C 2.129517 -0.031345 0.122631
C 2.613519 0.257622 1.414995
C 3.992530 0.220747 1.660865
C 0.678266 -0.003084 -0.137276
N -0.113884 -1.064113 -0.440705
C 0.075585 -2.532967 -0.187001
C -1.284153 -3.190043 -0.497402
N -0.126979 1.093702 -0.137218
Si -1.513076 0.050843 -0.665168
O -2.748195 -0.133389 0.364466
C -4.195633 0.023352 0.087457
C -4.646878 1.349891 0.694818
C 0.215624 2.548653 -0.295004
C -1.131736 3.265598 -0.517275
C 0.876096 3.086792 0.990015

C 1.134376 2.748085 -1.517005
C 1.158217 -3.111837 -1.119128
C 0.445658 -2.749418 1.294251
C -4.900122 -1.191728 0.685125
H 1.912766 0.491360 2.216906
H 4.367423 0.428714 2.663871
H 5.960002 -0.096236 0.812634
H 5.096576 -0.583735 -1.480194
H 2.639899 -0.563655 -1.917483
H -1.203754 -4.275691 -0.347300
H -2.069177 -2.804666 0.170758
H -1.574282 -3.011759 -1.546390
H 0.525796 -3.828705 1.492075
H 1.412188 -2.282467 1.531010
H -0.331399 -2.330071 1.952173
H 1.162104 -4.207345 -1.016452
H 0.942972 -2.862384 -2.169480
H 2.156724 -2.740763 -0.855206
H -0.959441 4.346233 -0.617517
H -1.618760 2.916779 -1.443598
H -1.806717 3.099282 0.336930
H 1.325312 3.822834 -1.654855
H 2.099136 2.241736 -1.374729
H 0.655204 2.361860 -2.430917
H 0.964853 4.180579 0.909494
H 0.260316 2.850618 1.871086
H 1.882636 2.671933 1.128167
H -4.332744 0.041168 -1.007745
H -5.982359 -1.115898 0.498957
H -4.532010 -2.123650 0.230664
H -4.731439 -1.230043 1.772000
H -5.725117 1.487643 0.520730
H -4.462349 1.351145 1.779802
H -4.110571 2.196250 0.238440
H -1.913135 0.257411 -2.073275

27-H$^+$
C -2.741599 0.112561 1.482686
C -4.042261 0.132630 2.004948
C -5.148034 0.108594 1.139346
C -4.955057 0.056848 -0.251366
C -3.658670 0.019756 -0.781193
C -2.550992 0.050977 0.087883
C -1.168255 0.014819 -0.436865
N -0.312147 1.068475 -0.503459
C -0.631596 2.533602 -0.591995
C -1.602607 2.776343 -1.767108
N -0.491441 -1.067142 -0.885302
Si 1.015343 -0.048135 -1.095929
P 2.642357 -0.843630 0.197170
C 4.182543 0.225861 -0.143520
C 3.954334 1.708452 -0.494552
C -0.779823 -2.533057 -0.741473
C -0.576319 -2.948465 0.730925
C -2.212514 -2.870188 -1.201202
C 0.230864 -3.256849 -1.653408

C 2.025292 -0.399309 1.948748
C 2.864436 -1.205961 2.966081
C 2.003948 1.094806 2.314812
C -1.236116 3.045768 0.731186
C 0.699102 3.256376 -0.868211
C 5.016201 -0.469241 -1.243424
H -1.876846 0.149440 2.146975
H -4.190402 0.172861 3.084994
H -6.159391 0.131029 1.547815
H -5.813529 0.040396 -0.924159
H -3.502196 -0.036145 -1.858737
H 0.506019 4.331414 -0.990488
H 1.405223 3.127839 -0.036270
H 1.164550 2.889781 -1.797453
H -1.332689 4.140433 0.672954
H -2.232028 2.622037 0.910807
H -0.581856 2.799069 1.580544
H -1.777347 3.857285 -1.875645
H -1.175670 2.397341 -2.709155
H -2.570120 2.288931 -1.585655
H 0.064533 -4.341486 -1.585550
H 0.095752 -2.950280 -2.702546
H 1.267027 -3.051978 -1.342467
H -2.302885 -3.965001 -1.260256
H -2.968657 -2.503109 -0.496990
H -2.411943 -2.452365 -2.199257
H -0.806152 -4.018870 0.843143
H 0.466104 -2.787310 1.044982
H -1.250988 -2.379660 1.389057
H 5.955774 0.085235 -1.399063
H 5.263229 -1.507869 -0.977929
H 4.471249 -0.478473 -2.202523
H 4.927876 2.212330 -0.614601
H 3.417652 1.804345 -1.453491
H 3.388045 2.240440 0.279685
H 4.736061 0.166215 0.810274
H 0.991021 -0.783153 1.971808
H 1.567481 1.218346 3.320412
H 3.022220 1.510724 2.346178
H 1.404244 1.679379 1.603285
H 2.494652 -1.009374 3.985556
H 2.809278 -2.288647 2.777498
H 3.923278 -0.901326 2.932341
H 1.349114 0.183237 -2.523084

28-H$^+$
C 3.463395 -0.573925 1.230411
C 4.798206 -0.791579 1.601712
C 5.832239 -0.557607 0.681541
C 5.535102 -0.094073 -0.611609
C 4.206625 0.141781 -0.985562
C 3.168978 -0.103193 -0.064099
C 1.759691 0.127481 -0.451054
N 0.833787 -0.826965 -0.724631
C 1.011007 -2.270537 -1.086176
C 2.187481 -2.458936 -2.066206

N 1.138026 1.320323 -0.586872
Si -0.428182 0.474892 -1.020056
P -2.143901 0.896963 0.267615
Si -3.962504 0.270939 -1.010491
C -3.734758 -1.405672 -1.876197
C 1.501597 2.682156 -0.078454
C 1.356145 2.689677 1.457344
C 2.932964 3.082261 -0.487961
C 0.495392 3.658740 -0.719807
Si -2.024896 -0.528308 2.069421
C -0.226615 -0.537687 2.688095
C -3.187228 0.232430 3.360393
C -2.589458 -2.292081 1.641272
C 1.231146 -3.104788 0.192026
C -0.298864 -2.698549 -1.775985
C -5.406849 0.194813 0.220833
C -4.196576 1.650016 -2.292338
H 2.656327 -0.749993 1.942027
H 5.027848 -1.144960 2.608000
H 6.869142 -0.734810 0.970955
H 6.337892 0.086828 -1.327731
H 3.968268 0.506887 -1.984836
H -0.253328 -3.769724 -2.018227
H -1.167002 -2.532108 -1.121144
H -0.447948 -2.140836 -2.714078
H 1.300972 -4.169115 -0.079092
H 2.165425 -2.813941 0.691696
H 0.393225 -2.977442 0.892785
H 2.190609 -3.502161 -2.416211
H 2.071870 -1.800113 -2.941243
H 3.153144 -2.255441 -1.586814
H 0.718299 4.680603 -0.380870
H 0.574559 3.631973 -1.818017
H -0.536996 3.418047 -0.421890
H 3.073133 4.145912 -0.244029
H 3.693124 2.505011 0.052154
H 3.081491 2.953130 -1.570605
H 1.597089 3.691180 1.845047
H 0.323748 2.441727 1.746301
H 2.046897 1.963657 1.912564
H -6.345944 -0.010584 -0.321301
H -5.269351 -0.606913 0.964157
H -5.533566 1.146073 0.762689
H -5.086593 1.443188 -2.911619
H -4.340605 2.629090 -1.807758
H -3.332246 1.731609 -2.972913
H -4.652545 -1.655304 -2.437264
H -2.903546 -1.389526 -2.599703
H -3.550114 -2.221269 -1.160030
H -3.189836 -0.385066 4.275277
H -2.869421 1.250443 3.638041
H -4.223704 0.290171 2.991532
H -0.141768 -1.189785 3.574576
H 0.453168 -0.926010 1.915262
H 0.111001 0.469950 2.976274
H -2.593201 -2.908377 2.557568

H -3.612429 -2.303996 1.232495
H -1.926544 -2.784772 0.913043
H -0.694275 0.609158 -2.474089

29-H$^+$
C 4.346024 -0.267602 0.452889
C 3.808230 -0.567883 -0.810264
C 2.424816 -0.504818 -1.018657
C 1.580368 -0.115754 0.041875
C 2.118342 0.198745 1.307579
C 3.501435 0.107317 1.510992
C 0.128544 -0.003761 -0.171944
N -0.742295 -1.025157 -0.415453
C -0.620090 -2.505880 -0.161051
C -2.015261 -3.095360 -0.447485
N -0.610204 1.138304 -0.158623
Si -2.083620 0.165298 -0.508226
Cl -3.462749 0.119608 0.986317
C -0.214248 2.586379 -0.273479
C -1.490525 3.327195 -0.721997
C 0.235458 3.104671 1.106845
C 0.897353 2.764175 -1.325667
C 0.411221 -3.136527 -1.117141
C -0.227099 -2.735336 1.311978
H 1.455918 0.484696 2.124921
H 3.917903 0.331105 2.493910
H 5.423567 -0.326465 0.612440
H 4.464994 -0.853018 -1.633037
H 2.000453 -0.731135 -1.996852
H -1.979595 -4.185503 -0.314564
H -2.771176 -2.697651 0.247527
H -2.323300 -2.890270 -1.486009
H -0.183111 -3.816803 1.508489
H 0.761393 -2.304951 1.526871
H -0.972526 -2.289044 1.988404
H 0.352437 -4.230644 -1.019573
H 0.191128 -2.869317 -2.161955
H 1.434396 -2.827954 -0.869546
H -1.281606 4.403694 -0.790831
H -1.822402 2.982963 -1.715179
H -2.304944 3.187893 0.008448
H 1.083418 3.840092 -1.458686
H 1.835452 2.290205 -1.009434
H 0.588273 2.344170 -2.295795
H 0.399198 4.190754 1.043315
H -0.536446 2.910962 1.866932
H 1.177622 2.633178 1.415931
H -2.713528 0.350144 -1.826250

30-H$^+$
C 4.693880 -0.131941 0.704147
C 4.260010 -0.406965 -0.604184
C 2.893215 -0.384297 -0.911411
C 1.960274 -0.063164 0.096439
C 2.392907 0.223656 1.407989
C 3.761105 0.176355 1.708791

C 0.521978 -0.008306 -0.221643
N -0.295477 -1.058811 -0.508024
C -0.120570 -2.536462 -0.283211
C -1.486829 -3.176185 -0.598600
N -0.248819 1.110379 -0.292960
Si -1.657552 0.090535 -0.761415
Br -3.310789 0.037479 0.673130
C 0.112895 2.568009 -0.375425
C -1.165527 3.285759 -0.854301
C 0.507501 3.081747 1.023714
C 1.251800 2.784504 -1.391489
C 0.948243 -3.100521 -1.240982
C 0.263674 -2.789209 1.188465
H 1.662995 0.458269 2.183323
H 4.096736 0.381906 2.726097
H 5.758574 -0.158217 0.940446
H 4.984395 -0.640781 -1.385459
H 2.549279 -0.592762 -1.924792
H -1.404568 -4.267458 -0.497848
H -2.262974 -2.829195 0.100763
H -1.796803 -2.955181 -1.633793
H 0.329912 -3.873981 1.359773
H 1.239603 -2.342269 1.424619
H -0.499454 -2.375404 1.865943
H 0.947102 -4.197794 -1.159861
H 0.721846 -2.829410 -2.283723
H 1.951543 -2.740527 -0.980143
H -0.975435 4.366635 -0.910837
H -1.461726 2.943236 -1.859784
H -1.997393 3.124045 -0.149266
H 1.424261 3.865519 -1.500933
H 2.187989 2.319202 -1.056403
H 0.977297 2.376687 -2.377326
H 0.647765 4.172026 0.975549
H -0.283944 2.862741 1.756620
H 1.449987 2.628842 1.358575
H -2.120891 0.225762 -2.154187

31-H$^+$

C	3.072007	-1.635711	-1.064541
C	2.638006	-0.683876	-0.112230
C	3.537771	-0.008619	0.753790
C	4.898323	-0.347962	0.673977
C	5.350184	-1.312630	-0.238286
C	4.447262	-1.936102	-1.104384
N	1.233040	-0.401240	0.043083
Si	-0.062738	0.483549	-0.923446
N	-0.515462	2.095166	-0.634670
Si	0.825730	3.325901	-0.780790
C	2.357515	2.490569	-1.541808
C	3.031522	1.057022	1.728604
C	4.078487	2.147841	2.029994
C	2.136621	-2.308898	-2.068847
C	2.201332	-3.850475	-1.988587
C	0.310894	-1.362741	0.370854
N	0.517995	-2.550220	0.952554

C	1.735274	-2.895543	1.709298
N	-0.891438	-0.895169	-0.094732
C	-2.172416	-1.239340	0.452629
C	-2.446838	-0.962819	1.813632
C	-3.717957	-1.319249	2.301771
C	-4.679290	-1.898722	1.466834
C	-4.380177	-2.158073	0.121764
C	-3.117663	-1.847522	-0.409181
C	-1.437548	-0.306290	2.758172
C	-0.963006	-1.311166	3.834313
C	-2.762102	-2.149582	-1.865612
C	-3.045254	-0.927837	-2.772292
C	-0.465728	-3.644989	0.833104
C	-3.474259	-3.399528	-2.424354
C	-1.998237	0.966319	3.434309
Si	-2.206229	2.786964	-0.671667
C	-2.648492	3.228606	-2.464240
C	-3.556932	1.610112	-0.070335
C	-2.243480	4.298130	0.475717
C	2.505142	0.440879	3.046473
C	2.456185	-1.819329	-3.501327
C	0.387083	4.725883	-1.981285
C	1.179398	4.042568	0.940907
H	-5.132446	-2.622909	-0.515470
H	-5.662731	-2.155345	1.864309
H	-3.957150	-1.123756	3.348372
H	4.809166	-2.664281	-1.831911
H	5.615510	0.150410	1.325749
H	-1.675904	-2.338720	-1.908787
H	-2.762552	-1.150094	-3.813526
H	-4.116809	-0.673351	-2.748476
H	-2.483268	-0.037905	-2.448055
H	-3.065101	-3.644589	-3.416353
H	-3.338963	-4.269703	-1.762957
H	-4.554796	-3.225471	-2.545828
H	-0.557972	0.014258	2.183428
H	-0.195294	-0.848381	4.474251
H	-1.804657	-1.616546	4.475602
H	-0.536110	-2.216359	3.377523
H	-1.236749	1.390297	4.108229
H	-2.264310	1.731043	2.690105
H	-2.893040	0.741464	4.034671
H	1.098016	-2.018147	-1.859596
H	1.759427	-2.275497	-4.222748
H	2.367838	-0.723761	-3.570560
H	3.481905	-2.098176	-3.789038
H	1.497831	-4.294278	-2.710587
H	3.209984	-4.219530	-2.229765
H	1.938339	-4.210612	-0.981669
H	2.175988	1.548550	1.247357
H	3.605822	2.960131	2.601892
H	4.908813	1.753553	2.636918
H	4.497818	2.567911	1.102784
H	2.200129	1.242008	3.739323
H	1.628104	-0.198280	2.868738
H	3.287508	-0.157881	3.540502

H	1.419766	-3.404586	2.632294
H	2.372680	-3.566018	1.113953
H	2.299595	-2.000586	1.971307
H	0.097531	-4.587620	0.784261
H	-1.144839	-3.661590	1.698261
H	-1.048325	-3.531234	-0.085854
H	1.229293	5.440389	-1.984634
H	0.267710	4.353497	-3.011244
H	-0.518757	5.287476	-1.714150
H	2.222265	4.393964	1.009554
H	0.521274	4.900611	1.149428
H	1.019590	3.301795	1.739495
H	3.122154	3.276261	-1.672190
H	2.826438	1.692967	-0.951503
H	2.144121	2.091522	-2.548550
H	-3.693021	3.582765	-2.510375
H	-2.011224	4.010258	-2.901215
H	-2.579689	2.337915	-3.112464
H	-3.275422	4.687934	0.507184
H	-1.962953	4.021254	1.505235
H	-1.590853	5.125268	0.161818
H	-4.493995	2.192771	-0.131907
H	-3.696149	0.717840	-0.693969
H	-3.447001	1.278259	0.969187
H	6.411238	-1.564019	-0.282984
H	0.178839	0.131747	-2.339399

32-H$^+$

C -4.006379 -1.390310 0.983821
C -3.840024 -0.719334 -0.243283
C -4.784412 -0.883239 -1.275231
C -5.894442 -1.715013 -1.075148
C -6.057702 -2.390685 0.145589
C -5.112625 -2.229664 1.172303
C -2.666794 0.159329 -0.445921
N -2.446806 1.365712 0.118396
C -3.313716 2.252277 0.945528
C -4.770441 2.246871 0.438114
N -1.585857 -0.099017 -1.219426
C -1.179332 -1.300294 -1.994908
C -1.482395 -2.611525 -1.240635
Si -0.798513 1.484869 -0.692546
Si 1.012699 1.820373 0.839607
N 2.427589 1.349283 -0.325792
C 3.353829 2.114500 -1.200040
C 2.582872 3.374849 -1.642033
N 1.518006 0.020964 1.102864
C 1.178328 -1.008953 2.112490
C 1.938730 -0.725344 3.426839
C 2.598302 0.166723 0.303291
C 3.767714 -0.747808 0.222586
C 3.850918 -1.724376 -0.788051
C 4.940593 -2.605479 -0.822389
C 5.951523 -2.514357 0.148428
C 5.874231 -1.536889 1.153746
C 4.784360 -0.655473 1.193777

C -0.341121 -0.871237 2.347755
C 1.492132 -2.435562 1.613349
C 4.617034 2.526633 -0.412798
C 3.732935 1.286720 -2.446412
C -1.892026 -1.290419 -3.364828
C 0.344161 -1.163476 -2.195621
C -3.247054 1.808211 2.422447
C -2.725020 3.671731 0.803900
H -3.261582 -1.271129 1.770812
H -5.236395 -2.757177 2.119359
H -6.920976 -3.040579 0.296952
H -6.631907 -1.833089 -1.870398
H -4.659877 -0.343385 -2.214407
H -3.308705 4.374007 1.416020
H -1.680316 3.701283 1.156702
H -2.763467 4.007478 -0.244071
H -3.827344 2.508553 3.042485
H -3.670146 0.801809 2.548646
H -2.205251 1.809154 2.778600
H -5.335204 3.012903 0.990336
H -4.807764 2.492853 -0.634337
H -5.258863 1.277545 0.600020
H 0.718973 -2.018108 -2.777679
H 0.586638 -0.241017 -2.748958
H 0.853358 -1.140198 -1.221343
H -1.503393 -2.110476 -3.988339
H -2.974294 -1.435681 -3.241037
H -1.714750 -0.337422 -3.886708
H -1.058025 -3.450321 -1.812863
H -1.022202 -2.604504 -0.241882
H -2.561198 -2.780141 -1.134589
H 4.317671 1.918428 -3.132325
H 4.341628 0.413320 -2.179887
H 2.827552 0.945881 -2.972824
H 5.254412 3.165445 -1.043541
H 4.335854 3.093562 0.488676
H 5.198405 1.643371 -0.114247
H 3.226087 3.997107 -2.280796
H 1.683784 3.102696 -2.218009
H 2.283402 3.978014 -0.768870
H -0.666043 -1.580253 3.123685
H -0.592958 0.146613 2.688501
H -0.892529 -1.081849 1.419184
H 1.057555 -3.157906 2.321065
H 1.052260 -2.611110 0.620367
H 2.572092 -2.618642 1.555646
H 1.627710 -1.442082 4.203105
H 3.021590 -0.831600 3.270559
H 1.725185 0.294574 3.782382
H 4.722204 0.109038 1.969577
H 6.661115 -1.459384 1.905754
H 6.798535 -3.201724 0.120088
H 5.000150 -3.362795 -1.605892
H 3.061262 -1.792379 -1.536514
H -0.928443 2.446898 -1.830145

33-H$^+$

C 5.287689 0.854656 0.083159
C 4.257162 0.253971 -0.680185
C 4.508136 -0.094147 -2.026398
C 5.758244 0.159037 -2.594510
C 6.792635 0.753500 -1.842742
C 6.533736 1.092771 -0.495817
C 2.947039 -0.009601 -0.101857
N 2.357836 0.609683 0.945111
C 2.745594 1.800791 1.639179
C 3.231376 1.661031 2.962448
C 3.626175 2.827231 3.640480
C 3.532196 4.085047 3.031405
C 3.020879 4.196872 1.732957
C 2.608728 3.061534 1.013654
C 3.342902 0.302999 3.653628
C 4.809279 -0.033009 4.009067
C 2.014588 3.217972 -0.379880
C 0.742779 4.097626 -0.346424
C 8.148623 1.025932 -2.453771
N 2.043238 -0.942392 -0.534289
C 2.372639 -2.219616 -1.109384
C 3.163607 -3.134974 -0.364215
C 3.419180 -4.395752 -0.930848
C 2.901325 -4.752983 -2.180460
C 2.121477 -3.836700 -2.893400
C 1.847430 -2.555860 -2.380113
C 3.749623 -2.824895 1.013058
C 3.257298 -3.829933 2.079825
C 1.001009 -1.593342 -3.209604
C 1.641693 -1.333745 -4.593402
Si 0.848980 -0.420863 0.790485
Si -1.064424 0.968893 1.109634
N -2.319377 -0.428809 1.078048
C -2.647533 -1.564825 1.877785
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C -3.503507 -2.465351 3.955022
C -3.246368 -3.763650 3.499299
C -2.681184 -3.957173 2.233556
C -2.359281 -2.869014 1.403648
C -3.534541 0.054153 3.687803
C -5.036890 0.209720 4.017755
C -1.738162 -3.124493 0.034478
C -0.469840 -4.003561 0.127679
N -2.045721 1.013520 -0.514500
C -2.873378 0.017655 -0.065973
C -4.121620 -0.419048 -0.682084
C -4.291036 -0.292310 -2.077163
C -5.473054 -0.723922 -2.684086
C -6.517746 -1.285808 -1.923250
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C -5.163121 -0.983608 0.091625
C -7.800609 -1.751321 -2.576334
C -2.502769 2.167532 -1.255957
C -3.406662 3.077039 -0.641550
C -3.745246 4.251105 -1.337577

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C -1.987181 2.411960 -2.553611
C -4.038280 2.851075 0.732159
C -3.617482 3.949914 1.734345
C -1.088330 1.424727 -3.297246
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C -5.578143 2.750828 0.626764
C -2.658870 0.390767 4.915967
C -2.771188 -3.765856 -0.922019
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H 5.940077 -0.106397 -3.637862
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H -3.488847 0.131924 -2.675778
H 8.191789 0.698144 -3.502476
H 8.384525 2.102763 -2.417253
H 8.942258 0.503470 -1.893897
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H -7.986822 -2.817081 -2.362330
H -8.665617 -1.188389 -2.186835
H 4.011690 2.742521 4.657939
H 3.847854 4.978772 3.572820
H 2.928486 5.179136 1.266596
H 4.029003 -5.108325 -0.373019
H 3.106222 -5.740940 -2.596846
H 1.718056 -4.111087 -3.869349
H -3.942855 -2.312455 4.942210
H -3.484711 -4.622692 4.129216
H -2.478778 -4.969297 1.879397
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H -6.009140 3.698803 0.267873
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H -1.007208 0.507491 -2.695995
H -1.028264 0.342844 -5.197571
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H -1.783468 1.945800 -5.313397
H 0.967864 1.290290 -4.039529
H 0.287717 2.938088 -4.076715
H 0.801762 2.227147 -2.531423
H -1.436062 -2.153123 -0.390745

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H 0.271005 -3.566013 0.813641
H -0.716665 -5.011989 0.494517
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H -3.660799 -3.129775 -1.034256
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H -5.661180 0.020154 3.129948
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H -2.881045 1.408987 5.273485
H -2.851813 -0.314969 5.739723
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H 2.986844 -0.473019 2.961650
H 2.506963 -0.746429 5.378134
H 2.760258 0.998250 5.652770
H 1.390855 0.449979 4.652255
H 4.862813 -1.019176 4.497983
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H 5.227473 0.714461 4.701662
H 1.716108 2.221213 -0.735763
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H 3.946985 3.138975 -1.421234
H 0.280082 4.142881 -1.343923
H 0.000851 3.694146 0.362209
H 0.987480 5.124516 -0.032192
H 3.413903 -1.834197 1.342908
H 3.660141 -3.552950 3.067425
H 2.157908 -3.837961 2.139406
H 3.596212 -4.851680 1.848576
H 5.699343 -2.514976 1.946734
H 5.695258 -3.779602 0.688242
H 5.649339 -2.058653 0.217856
H 0.940336 -0.632953 -2.677729
H -1.032089 -1.473687 -4.014775
H -0.413863 -3.136420 -3.854617
H -0.935217 -2.238175 -2.409669
H 1.018989 -0.636131 -5.174553
H 2.649424 -0.898577 -4.500568
H 1.728562 -2.268099 -5.169443
H 0.933216 -1.465158 1.856071

34-H$^+$
C 4.855625 -1.562686 1.450492
C 5.049836 -1.363207 0.068356
C 6.274085 -1.715703 -0.537821
C 7.294731 -2.279111 0.238949
C 7.107629 -2.466959 1.619352
C 5.892684 -2.102738 2.223623
C 3.970036 -0.784234 -0.753147
N 3.980766 0.424255 -1.371990
C 4.723740 1.680125 -1.002963
C 6.242244 1.496407 -1.195647
N 2.774087 -1.365257 -1.048632
C 2.427754 -2.831091 -1.109766

C 2.357536 -3.438658 0.304380
Si 2.328797 0.082827 -2.048961
C 1.055839 1.348997 -1.505654
C -0.351274 0.873979 -1.136447
C -0.965207 -0.065187 -1.993939
C -2.105696 -0.851741 -1.686036
C -2.361017 -2.086444 -2.529709
N -2.922059 -0.568059 -0.669403
Ge -3.030672 1.373720 0.062647
N -0.939170 1.386642 -0.050275
C -0.272239 2.353139 0.780975
C -0.205213 3.706155 0.352549
C 0.447910 4.633286 1.185730
C 1.018138 4.239898 2.401229
C 0.926252 2.903630 2.812346
C 0.269589 1.940917 2.024522
C -0.830403 4.191271 -0.954880
C -2.043292 5.106830 -0.662920
C 0.204746 0.485486 2.479112
C 1.526087 -0.229136 2.123851
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Cl -3.286983 0.850685 2.252572
C 0.195159 4.927049 -1.849450
C -0.100744 0.336067 3.983132
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37-H$^+$
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38-H$^+$
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H -5.452796 -1.051796 2.509969
H -4.104152 -1.523859 3.589309
H -5.152399 1.961173 2.521634
H -3.883115 2.149014 1.274438
H -5.230355 0.994626 1.023322
H -3.371191 1.479653 4.266579
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H -3.696686 -2.661754 -2.179071
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H -0.565260 -0.606969 -2.404721
H -0.179075 -3.752768 -1.791753
H 0.408298 -2.455526 -0.720458
H -0.739077 -3.674329 -0.097219

H -2.520386 1.357623 -1.625464
H -2.743142 4.057109 -1.768590
H -1.460192 5.113837 0.381168
H -0.470375 3.080909 1.849779
H 0.063261 1.295436 -3.187192
H -0.006782 3.962913 -3.561874
H 1.358426 5.142792 -1.535158
H 2.314359 3.192611 0.077962
H -0.387159 -0.503481 2.012600

39-H$^+$
C 3.048014 -1.934909 -0.353730
C 3.600002 -0.926962 0.454080
C 4.845843 -1.144438 1.068546
C 5.532703 -2.354267 0.881859
C 4.972883 -3.356861 0.075377
C 3.727494 -3.144062 -0.542383
C 2.895979 0.395460 0.664610
N 1.484239 0.330007 1.200124
C 1.195359 0.104770 2.633171
C -0.338281 0.181214 2.779410
Si 1.040638 1.651835 0.144685
N 2.535976 1.153356 -0.585124
C 3.527880 1.845537 -1.434420
C 4.451939 2.754487 -0.592194
Si -0.923305 1.431213 -1.144442
N -1.617344 -0.228483 -1.421515
C -0.995390 -1.538659 -1.800875
C -1.978083 -2.397213 -2.620220
C -2.633519 0.045052 -0.562559
N -2.455399 1.326025 -0.156748
C -3.424420 2.311265 0.416987
C -3.878201 1.885775 1.828032
C -3.718430 -0.871809 -0.157545
C -4.709226 -1.230937 -1.093612
C -5.744344 -2.094512 -0.711269
C -5.781446 -2.614774 0.593163
C -4.787672 -2.263667 1.521960
C -3.759892 -1.384943 1.154399
C -2.658792 3.646678 0.500660
C -4.634286 2.445167 -0.530979
C 0.218645 -1.168766 -2.678051
C -0.555432 -2.273225 -0.517776
C 4.372118 0.813745 -2.214554
C 2.721379 2.703482 -2.430627
C 1.677972 -1.300088 3.052775
C 1.854458 1.177285 3.532179
H -2.990433 -1.099820 1.872043
H -4.813696 -2.670923 2.533701
H -6.584011 -3.293524 0.885653
H -6.517295 -2.363617 -1.432458
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H -4.503135 0.984715 1.793064
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H 0.753421 -2.083002 -2.972413
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H -2.360949 -1.833997 -3.484954
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H -1.436126 -2.557992 0.077182
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H 4.963909 0.188523 -1.532236
H 3.719306 0.155408 -2.807596
H 5.143440 3.306702 -1.247053
H 3.860197 3.482871 -0.013691
H 5.055754 2.156782 0.107990
H 3.398902 3.216711 -3.128650
H 2.037073 2.068334 -3.017625
H 2.135903 3.477995 -1.902002
H -0.629897 0.029460 3.829657
H -0.716819 1.169668 2.463016
H -0.815531 -0.595087 2.161352
H 1.388173 -1.493528 4.097279
H 1.231840 -2.071079 2.407116
H 2.770880 -1.380758 2.974828
H 1.595964 1.005056 4.588795
H 2.951225 1.141910 3.444700
H 1.513108 2.186730 3.249852
H 0.885615 3.033321 0.724755
H 5.278449 -0.359575 1.695508
H 6.499828 -2.512431 1.362411
H 5.503774 -4.298938 -0.073585
H 3.292501 -3.922433 -1.173396
H 2.090037 -1.759173 -0.833565
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H -1.104503 2.293825 -2.344394

40-H$^+$
C -3.871397 -1.202755 1.259139
C -3.755559 -1.016246 -0.134259
C -4.689810 -1.604466 -1.010626
C -5.738095 -2.373665 -0.490295
C -5.846804 -2.571559 0.896472
C -4.910347 -1.991826 1.768851
C -2.683329 -0.153640 -0.660725
N -2.515074 1.166146 -0.402120
C -3.461826 2.217094 0.101603
C -4.923254 1.879410 -0.254984
N -1.653716 -0.519188 -1.475787
C -1.033908 -1.863744 -1.719388
C -0.622820 -2.485563 -0.369728

Si -0.941242 1.145322 -1.317228
Si 0.974646 1.377224 0.022734
Cl 0.683656 3.358774 0.745459
N 1.452609 0.164347 1.160642
C 1.129679 -0.114766 2.577325
C 1.814105 0.898208 3.523719
C 2.866618 0.239665 0.637665
N 2.505021 0.952104 -0.639266
C 3.486628 1.594535 -1.539085
C 2.673787 2.420177 -2.556562
C 3.588053 -1.078436 0.470633
C 3.029444 -2.135701 -0.266137
C 3.727595 -3.338678 -0.419268
C 4.997474 -3.496081 0.164623
C 5.561514 -2.445124 0.903381
C 4.856011 -1.240782 1.055292
C -0.401978 0.006334 2.704681
C 1.560977 -1.550650 2.947461
C 4.431567 2.523958 -0.744473
C 4.305931 0.521641 -2.289864
C -2.000965 -2.791669 -2.480566
C 0.196785 -1.582951 -2.607072
C -3.289003 2.365343 1.626645
C -3.051489 3.527147 -0.602941
H -3.141007 -0.748735 1.928381
H -4.991136 -2.150090 2.845160
H -6.661953 -3.176152 1.296987
H -6.470031 -2.817132 -1.166662
H -4.603083 -1.439657 -2.084563
H -3.682628 4.349466 -0.237128
H -2.002942 3.784166 -0.380239
H -3.185419 3.444418 -1.692811
H -3.945386 3.171841 1.986978
H -3.565782 1.436030 2.143823
H -2.250306 2.625727 1.877300
H -5.545084 2.751845 -0.005920
H -5.027938 1.676963 -1.332038
H -5.299573 1.018123 0.310609
H 0.733561 -2.522440 -2.800613
H -0.115241 -1.158701 -3.574734
H 0.905223 -0.891680 -2.118546
H -1.447559 -3.689854 -2.793637
H -2.837223 -3.111866 -1.846890
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H -0.101894 -3.439085 -0.545035
H 0.051850 -1.811582 0.178468
H -1.513276 -2.686214 0.244856
H 4.987608 1.014506 -3.000359
H 4.904614 -0.082276 -1.594963
H 3.637275 -0.151756 -2.847624
H 5.128085 3.029232 -1.431152
H 3.856766 3.288053 -0.198320
H 5.030509 1.947317 -0.022530
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H 2.108494 3.223067 -2.053768

H -0.710993 -0.197003 3.740950
H -0.740162 1.022366 2.443702
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H 1.102840 -2.284583 2.268029
H 2.651933 -1.663950 2.888535
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H 2.909781 0.829130 3.442629
H 1.506380 1.927127 3.283512
H 5.291772 -0.418682 1.629794
H 6.546050 -2.561155 1.359781
H 5.542745 -4.433888 0.043865
H 3.287138 -4.156479 -0.993970
H 2.047882 -2.006604 -0.712233
H 3.480348 0.893954 1.283831
H -0.978700 1.923601 -2.580580

41-H$^+$

C	-3.895143	0.517018	-1.390323
C	-3.531160	-0.189014	-0.226385
C	-4.474280	-1.004275	0.431059
C	-5.779296	-1.099376	-0.069067
C	-6.139444	-0.403550	-1.235542
C	-5.196266	0.398595	-1.898323
C	-2.155968	-0.068347	0.303122
N	-1.573602	1.020304	0.814329
C	-2.205858	2.227419	1.397184
C	-2.751802	3.183604	0.319991
N	-1.233956	-1.070991	0.381378
C	-1.097296	-2.273134	-0.477731
C	-2.232339	-3.293336	-0.289444
Si	-0.000041	0.000142	1.186408
N	1.233866	1.071016	0.381096
C	1.097342	2.273034	-0.478217
C	2.231683	3.293808	-0.288785
N	1.573504	-1.020133	0.814695
C	2.205718	-2.227218	1.397607
C	2.751318	-3.183674	0.320470
C	2.155896	0.068347	0.303158
C	3.531082	0.188901	-0.226380
C	4.474120	1.004470	0.430797
C	5.779157	1.099482	-0.069306
C	6.139408	0.403249	-1.235498
C	5.196312	-0.399209	-1.898024
C	3.895177	-0.517535	-1.390048
C	3.274907	-1.868433	2.446645
C	0.917579	1.866300	-1.952312
C	-0.916000	-1.866467	-1.951655
C	-3.274739	1.868694	2.446551
H	-0.163235	-2.733640	-0.127271
H	-1.372161	2.733833	1.909406
H	-3.157638	1.142931	-1.894368
H	-5.473456	0.934660	-2.807214
H	-7.154302	-0.486984	-1.627536
H	-6.512828	-1.719343	0.448430
H	-4.183658	-1.547261	1.330890

H	-0.740062	-2.759259	-2.571356
H	-1.820718	-1.361349	-2.324403
H	-0.056551	-1.186744	-2.063854
H	-1.947635	-4.234190	-0.785187
H	-2.401646	-3.499673	0.778117
H	-3.170411	-2.940361	-0.737904
H	-3.625580	2.785751	2.943806
H	-4.138035	1.381215	1.970714
H	-2.860044	1.194007	3.211571
H	-3.000738	4.148638	0.787147
H	-2.004510	3.361192	-0.469122
H	-3.663656	2.778391	-0.139918
H	1.372077	-2.733428	1.910119
H	3.625802	-2.785459	2.943917
H	4.138113	-1.381086	1.970509
H	2.860470	-1.193615	3.211689
H	3.000129	-4.148685	0.787739
H	2.003892	-3.361231	-0.468523
H	3.663198	-2.778711	-0.139612
H	0.162705	2.733027	-0.128645
H	1.947080	4.234521	-0.784853
H	2.399749	3.500247	0.778956
H	3.170389	2.941242	-0.736244
H	0.741577	2.759024	-2.572092
H	1.822903	1.361781	-2.324370
H	0.058641	1.186043	-2.065249
H	3.157736	-1.143649	-1.893930
H	5.473582	-0.935585	-2.806708
H	7.154278	0.486608	-1.627477
H	6.512615	1.719699	0.447998
H	4.183436	1.547748	1.330431
H	-0.000265	0.000215	2.666930

42-H$^+$

C	-2.748854	-1.541246	2.640591
C	-1.875346	-2.122510	1.516314
C	-2.528704	-3.370053	0.882047
N	-1.401312	-1.080947	0.556663
C	-2.056722	0.034159	0.127484
N	-3.365188	0.160268	-0.213871
C	-4.086694	1.421387	0.156306
C	-4.835869	1.264587	1.497549
Si	0.162624	-0.050992	0.843081
N	-1.102448	1.034667	0.117543
C	-0.899352	2.141652	-0.865162
C	-1.409184	3.521601	-0.392068
N	1.444348	-1.037200	0.009813
C	1.420014	-2.069329	-1.050350
C	0.425986	-1.684893	-2.163844
C	2.378820	-0.037301	0.093995
N	1.731497	1.039302	0.588668
C	2.381174	2.126473	1.348853
C	2.160150	3.484832	0.658094
N	3.702947	-0.148271	-0.217760
C	4.550377	-1.275732	0.297130
C	4.709904	-2.500179	-0.630457

C	4.361340	0.980574	-0.947279
C	5.603220	1.565569	-0.243765
C	1.850656	2.162179	2.794410
C	1.109612	-3.443708	-0.444287
C	-4.034058	-0.988849	-0.901951
C	-5.365497	-1.426803	-0.273407
C	-1.410386	1.793316	-2.271490
C	4.713665	0.541062	-2.382407
C	4.109044	-1.697502	1.709559
C	-4.186215	-0.731554	-2.417567
C	-5.015181	1.984112	-0.930869
H	-0.930261	-2.464259	1.969763
H	0.196030	2.216678	-0.912177
H	-2.414601	-4.218832	1.573754
H	-3.605506	-3.231398	0.712579
H	-2.048285	-3.636612	-0.070750
H	-2.928581	-2.310798	3.407046
H	-2.252200	-0.682292	3.118082
H	-3.720450	-1.213221	2.249514
H	-0.825226	4.306998	-0.896657
H	-2.465632	3.693683	-0.647208
H	-1.279334	3.639204	0.694134
H	-1.120305	2.593088	-2.970164
H	-0.978334	0.845532	-2.625098
H	-2.502799	1.703724	-2.288919
H	2.421564	-2.079446	-1.495130
H	1.114433	-4.217023	-1.228006
H	1.853651	-3.713133	0.320381
H	0.116858	-3.431973	0.026665
H	0.465511	-2.429605	-2.974198
H	-0.599526	-1.645330	-1.769875
H	0.687360	-0.700894	-2.584858
H	3.458115	1.911408	1.384023
H	2.348509	2.971762	3.349642
H	0.766194	2.355425	2.803918
H	2.039478	1.209762	3.311537
H	2.720555	4.270462	1.187855
H	2.493476	3.467187	-0.390910
H	1.093272	3.752146	0.676284
H	3.599520	1.766819	-1.010484
H	5.088150	1.405231	-2.953293
H	5.503777	-0.224668	-2.372232
H	3.830335	0.133010	-2.897129
H	5.848636	2.529950	-0.713327
H	5.437771	1.734357	0.830145
H	6.482817	0.913831	-0.361312
H	5.544507	-0.820940	0.394166
H	4.819884	-2.439547	2.102463
H	4.092081	-0.832152	2.390130
H	3.108448	-2.153158	1.691303
H	5.634603	-3.030493	-0.353237
H	3.879670	-3.211067	-0.517144
H	4.787532	-2.205236	-1.685635
H	-3.327560	-1.817134	-0.811799
H	-3.298908	2.153843	0.336342
H	-5.392622	2.957387	-0.582463

H	-4.496734	2.139931	-1.885968
H	-5.883938	1.334910	-1.104848
H	-5.254875	2.242659	1.781937
H	-5.663027	0.546777	1.429400
H	-4.147341	0.942201	2.290848
H	-5.703837	-2.341721	-0.783071
H	-5.260957	-1.647394	0.797456
H	-6.147955	-0.666156	-0.399785
H	-4.488984	-1.674801	-2.899131
H	-4.951066	0.021752	-2.642921
H	-3.229801	-0.412027	-2.854941
H	0.208864	-0.160315	2.318183

43-H$^+$

C 2.937009 0.005042 -0.050925
Si 4.814428 -0.081856 -0.139683
C 5.547295 -0.345923 1.598496
P 1.932365 1.402975 0.277099
C 1.926969 2.674506 -1.081702
C 2.493362 2.404213 1.739550
P 1.812209 -1.321422 -0.097428
C 2.197868 -2.751636 1.024050
Si -0.000022 0.000057 0.580477
P -1.812238 1.321413 -0.097624
C -1.617451 2.159305 -1.745268
C -2.937032 -0.005045 -0.051007
Si -4.814459 0.081833 -0.139571
C -5.547187 0.345735 1.598691
C -2.197843 2.751656 1.023835
C 1.617472 -2.159445 -1.745027
C 5.305783 -1.542605 -1.261451
C 5.471477 1.558043 -0.853425
P -1.932310 -1.402936 0.277001
C -1.926768 -2.674369 -1.081892
C -2.493387 -2.404257 1.739361
C -5.305932 1.542637 -1.261206
C -5.471571 -1.557978 -0.853477
H 6.403380 -1.633427 -1.324786
H 4.927799 -2.506296 -0.876618
H 4.923660 -1.413973 -2.288130
H 6.649600 -0.394098 1.567431
H 5.270319 0.476441 2.280022
H 5.187252 -1.285352 2.052113
H 6.573688 1.548118 -0.898640
H 5.098210 1.739562 -1.875194
H 5.184367 2.422433 -0.229221
H -6.573806 -1.548197 -0.898209
H -5.098738 -1.739096 -1.875476
H -5.184072 -2.422557 -0.229714
H -6.649492 0.393950 1.567697
H -5.270196 -0.476711 2.280109
H -5.187087 1.285101 2.052392
H -6.403535 1.633655 -1.324169
H -4.927635 2.506287 -0.876580
H -4.924180 1.413861 -2.288007
H 2.302518 -2.387606 2.056085

H 1.398033 -3.508554 0.977493
H 3.143386 -3.223298 0.711734
H 2.598623 -2.546415 -2.062179
H 0.903500 -2.995299 -1.688126
H 1.271862 -1.428343 -2.490900
H 1.314730 3.547471 -0.802321
H 2.958842 3.011469 -1.265542
H 1.532817 2.228904 -2.006394
H 1.824262 3.264953 1.900682
H 2.492321 1.768386 2.636726
H 3.514954 2.780870 1.570008
H -1.824582 -3.265263 1.900264
H -2.492020 -1.768587 2.636651
H -3.515141 -2.780492 1.569887
H -1.314507 -3.547326 -0.802517
H -2.958612 -3.011369 -1.265823
H -1.532555 -2.228701 -2.006524
H -0.903475 2.995161 -1.688384
H -1.271814 1.428146 -2.491068
H -2.598575 2.546284 -2.062494
H -3.143183 3.223587 0.711388
H -2.302787 2.387514 2.055802
H -1.397820 3.508391 0.977542
H -0.000332 0.000230 2.078536

44-H$^+$
C 3.073148 1.532863 -0.136665
C 2.766102 0.030649 -0.020255
C 3.359198 -0.726245 -1.229458
N 1.262719 -0.151610 -0.050346
C 0.701831 -1.379448 0.010324
C -0.701886 -1.379436 0.010315
N -1.262772 -0.151633 -0.050361
C -2.766147 0.030657 -0.020277
C -3.311336 -0.528756 1.310584
Si -0.000026 1.104027 0.179184
C 3.311431 -0.528741 1.310525
C -3.073009 1.532920 -0.136654
C -3.359308 -0.726184 -1.229416
H 1.312637 -2.272889 0.121865
H -1.312703 -2.272918 0.121508
H 4.447539 -0.571399 -1.238269
H 3.169184 -1.807612 -1.161155
H 2.940504 -0.346634 -2.173105
H 4.162593 1.675373 -0.134030
H 2.678515 1.951569 -1.075338
H 2.666109 2.094976 0.722040
H 4.401498 -0.386900 1.336355
H 2.867002 0.002182 2.166019
H 3.105535 -1.605160 1.409452
H -4.162427 1.675582 -0.133901
H -2.665851 2.094968 0.722055
H -2.678347 1.951580 -1.075336
H -4.401437 -0.387186 1.336442
H -3.105114 -1.605114 1.409512
H -2.866987 0.002329 2.166014

H -4.447669 -0.571450 -1.238056
H -2.940836 -0.346469 -2.173123
H -3.169235 -1.807552 -1.161252
H 0.000077 2.049375 -0.965466

45-H$^+$
C 3.323393 -1.250381 0.094899
C 2.697960 0.020585 0.107709
C 3.425858 1.225479 -0.059549
C 4.815229 1.124743 -0.231635
C 5.481919 -0.112930 -0.222183
C 4.716630 -1.283682 -0.057474
N 1.264478 0.074912 0.271543
Si -0.001446 -0.332901 -0.957232
N -1.264186 0.077238 0.273458
C -0.699776 0.768933 1.292995
C 0.702512 0.767836 1.291768
C 2.757682 2.586250 -0.116538
C 6.985413 -0.189010 -0.370197
C 2.552292 -2.545177 0.273630
C -2.697937 0.022400 0.111321
C -3.323122 -1.248737 0.107298
C -4.717155 -1.282828 -0.037573
C -5.482622 -0.113326 -0.210095
C -4.817278 1.125053 -0.218602
C -3.427036 1.226698 -0.054015
C -2.551678 -2.541855 0.296598
C -2.760594 2.588447 -0.108023
C -6.980723 -0.193982 -0.404095
H -1.322420 1.288215 2.017991
H 1.327193 1.286559 2.015405
H -5.394516 2.041191 -0.363034
H -5.221135 -2.251727 -0.008273
H -3.222838 -3.330972 0.664217
H -2.119580 -2.898504 -0.653618
H -1.726791 -2.429107 1.016819
H -2.606875 3.014085 0.898240
H -1.776532 2.545382 -0.603370
H -3.391864 3.294594 -0.665433
H -7.419297 -0.992139 0.214426
H -7.469933 0.757939 -0.150083
H -7.222196 -0.424347 -1.456425
H 5.219940 -2.253289 -0.043190
H 5.390202 2.040727 -0.385322
H 3.387251 3.291462 -0.677073
H 1.772706 2.540791 -0.609947
H 2.605323 3.014690 0.888745
H 1.728022 -2.438458 0.995409
H 2.119655 -2.893982 -0.679245
H 3.223770 -3.337236 0.634263
H 7.386633 0.711848 -0.857515
H 7.466876 -0.276871 0.619407
H 7.283481 -1.070713 -0.958189
H -0.004680 -1.801675 -1.185406

46-H$^+$

C -3.317830 1.273855 0.047409
C -2.697201 0.002017 0.064252
C -3.413446 -1.210154 -0.095181
C -4.805171 -1.117487 -0.269653
C -5.452555 0.124739 -0.271390
C -4.713683 1.305122 -0.110317
N -1.259955 -0.047545 0.234999
C -0.701535 -0.678424 1.296411
C 0.701500 -0.678421 1.296440
N 1.260010 -0.047548 0.235074
Si 0.000002 0.293291 -1.007952
C -2.731903 -2.564648 -0.125342
C -2.542044 2.565941 0.223508
C 2.697200 0.002020 0.064380
C 3.413476 -1.210201 -0.094837
C 4.805156 -1.117586 -0.269444
C 5.452556 0.124654 -0.271512
C 4.713710 1.305061 -0.110631
C 3.317853 1.273838 0.047200
C 2.731764 -2.564615 -0.124793
C 2.542153 2.566013 0.223060
H -6.534551 0.174244 -0.400735
H 6.534542 0.174114 -0.400950
H -1.328333 -1.158057 2.045041
H 1.328255 -1.157972 2.045161
H -5.221180 2.271373 -0.100832
H -5.379056 -2.035141 -0.410321
H -3.361033 -3.291730 -0.657509
H -1.754433 -2.522133 -0.633945
H -2.560465 -2.963297 0.889092
H -2.100450 2.905916 -0.728615
H -3.212272 3.363786 0.573300
H -1.723876 2.460797 0.952549
H 5.379037 -2.035268 -0.409942
H 5.221207 2.271314 -0.101372
H 3.212261 3.363654 0.573552
H 2.101361 2.906313 -0.729322
H 1.723418 2.460847 0.951452
H 2.558396 -2.962252 0.889704
H 1.755184 -2.522322 -0.635151
H 3.361645 -3.292355 -0.655156
H -0.000061 1.737417 -1.352557

47-H$^+$
C 3.433377 -1.209312 -0.059073
C 2.688433 -0.008854 0.054656
C 3.271045 1.280724 -0.017306
C 4.662801 1.341472 -0.204875
C 5.432576 0.177123 -0.313032
C 4.821844 -1.080523 -0.239387
N 1.252217 -0.082706 0.235802
Si 0.000009 0.087411 -1.040583
N -1.252201 -0.082706 0.235773
C -0.702678 -0.574489 1.370234
C 0.702672 -0.574495 1.370247
C 2.470157 2.573549 0.136582

C 2.462140 3.377393 -1.184545
C 2.803088 -2.601019 -0.022706
C 3.225012 -3.359219 1.258676
C -2.688439 -0.008873 0.054667
C -3.433346 -1.209343 -0.059082
C -4.821852 -1.080585 -0.239171
C -5.432630 0.177043 -0.312629
C -4.662872 1.341412 -0.204504
C -3.271094 1.280698 -0.017121
C -2.803029 -2.601054 -0.023073
C -3.164069 -3.418812 -1.285541
C -2.470204 2.573525 0.136733
C -3.012086 3.437633 1.299934
C -2.462235 3.377329 -1.184424
C -3.225149 -3.359777 1.257918
C 3.012096 3.437612 1.299795
C 3.164376 -3.419346 -1.284722
H -6.512084 0.249780 -0.454370
H 6.512006 0.249874 -0.454945
H -1.335285 -0.959389 2.167847
H 1.335252 -0.959422 2.167867
H -5.146316 2.317736 -0.253626
H -5.426927 -1.982932 -0.333177
H -1.705824 -2.502850 -0.008541
H -1.427954 2.320765 0.384265
H 5.426939 -1.982853 -0.333421
H 5.146200 2.317812 -0.254137
H 1.427914 2.320794 0.384147
H 1.705876 -2.502811 -0.008447
H -2.388583 4.337882 1.415290
H -4.044630 3.763885 1.102426
H -3.004151 2.879106 2.248667
H -1.859791 4.292028 -1.066332
H -2.044216 2.786050 -2.015485
H -3.484726 3.674472 -1.465031
H -2.747415 -4.351595 1.285253
H -2.942947 -2.808611 2.169972
H -4.316608 -3.503215 1.278359
H -2.654713 -4.394558 -1.254432
H -4.247464 -3.604820 -1.340008
H -2.859797 -2.891510 -2.202959
H 2.388644 4.337894 1.415171
H 3.004141 2.879069 2.248519
H 4.044659 3.763803 1.102277
H 1.859723 4.292101 -1.066392
H 3.484619 3.674525 -1.465204
H 2.044057 2.786149 -2.015601
H 2.654948 -4.395043 -1.253278
H 2.860348 -2.892447 -2.202451
H 4.247766 -3.605481 -1.338864
H 2.747286 -4.351029 1.286365
H 4.316476 -3.502620 1.279285
H 2.942731 -2.807690 2.170487
H 0.000010 1.470401 -1.581869

48-H$^+$

C 3.050972 1.626112 0.039752
C 2.790694 0.109946 0.010462
C 3.389175 -0.549857 1.271613
C 3.397010 -0.507299 -1.268040
N 1.308445 -0.112478 0.006972
Si -0.000015 0.933295 -0.000114
N -1.308452 -0.112498 -0.007205
C -2.790696 0.109953 -0.010407
C -3.389399 -0.549968 -1.271405
C 0.756255 -1.492006 -0.189565
C -0.756239 -1.491997 0.189472
C -3.396807 -0.507178 1.268242
C -3.050950 1.626112 -0.039782
H 1.300139 -2.201061 0.447751
H -1.300121 -2.201120 -0.447775
H 4.479073 -0.313153 -1.282430
H 3.249435 -1.597047 -1.296541
H 2.948241 -0.060680 -2.168881
H 4.133678 1.810630 0.065753
H 2.647752 2.117834 -0.861730
H 2.613161 2.088896 0.940962
H 4.474834 -0.374369 1.288438
H 2.948717 -0.118430 2.183207
H 3.227096 -1.638119 1.275712
H -4.133655 1.810647 -0.065759
H -2.647696 2.117889 0.861655
H -2.613168 2.088839 -0.941036
H -4.478862 -0.313000 1.282763
H -3.249253 -1.596926 1.296829
H -2.947910 -0.060493 2.168989
H -4.475071 -0.374553 -1.288076
H -2.949101 -0.118589 -2.183100
H -3.227224 -1.638215 -1.275430
H -0.898739 -1.781524 1.242358
H 0.898751 -1.781632 -1.242423
H 0.000105 2.399963 -0.000062

49-H$^+$
C -3.198821 -1.664685 -0.222041
C -2.898391 -0.174381 0.016492
C -3.474017 0.264580 1.380066
C -3.496710 0.673337 -1.126233
N -1.410505 0.009264 0.040786
Si -0.130618 -1.039555 -0.195085
N 1.219575 -0.055771 -0.049113
C 2.671515 -0.450875 0.041179
C 3.435674 0.054758 -1.203042
C -0.823763 1.379737 0.105787
C 0.725177 1.313281 0.369778
C 1.397118 2.487675 -0.353352
C 3.280434 0.109936 1.343418
C 2.753479 -1.991090 0.073226
H -1.302684 1.953708 0.910385
H -4.582736 0.506085 -1.166888
H -3.326978 1.747681 -0.961811
H -3.060941 0.384938 -2.095528

H -4.286281 -1.821419 -0.218341
H -2.814709 -1.998389 -1.200761
H -2.768038 -2.291991 0.576919
H -4.562549 0.107469 1.378485
H -3.034156 -0.326949 2.197215
H -3.292216 1.332505 1.571769
H 3.806855 -2.294845 0.146927
H 2.221639 -2.403797 0.947631
H 2.350924 -2.437366 -0.852136
H 4.324646 -0.225798 1.417240
H 3.278353 1.208123 1.362010
H 2.732695 -0.262941 2.222943
H 4.472519 -0.311279 -1.157411
H 2.969400 -0.333872 -2.121325
H 3.464086 1.148920 -1.258058
H 0.909110 1.394042 1.452887
H -1.017916 1.890291 -0.851708
H 0.868701 3.414941 -0.079730
H 2.448138 2.605531 -0.063556
H 1.333164 2.357534 -1.443780
H -0.196037 -2.477437 -0.475579

50-H$^+$
C -3.399999 -1.535253 -0.957811
C -3.001286 -0.439999 0.046662
N -1.507531 -0.377314 0.102242
C -0.820241 0.475776 1.127106
C 0.668193 0.725193 0.694681
C 0.855373 2.055789 -0.125668
C 2.328372 2.235254 -0.545916
C -3.532132 -0.790597 1.453412
C -3.559151 0.922241 -0.418448
Si -0.287576 -1.172612 -0.714548
N 1.112299 -0.520976 -0.052999
C 2.417245 -1.283973 0.135986
C 2.072020 -2.677302 0.718955
C 3.094813 -1.456427 -1.239149
C 3.362369 -0.574611 1.119053
C -0.027446 2.090202 -1.389982
C 0.484950 3.247925 0.794255
H -0.867108 -0.037396 2.100590
H -4.657695 0.871996 -0.441640
H -3.276452 1.733134 0.269294
H -3.198534 1.166684 -1.428553
H -4.495446 -1.600482 -1.013266
H -3.028547 -1.301823 -1.970440
H -3.017271 -2.520690 -0.643271
H -4.627671 -0.874726 1.413179
H -3.118001 -1.750377 1.798902
H -3.278761 -0.007763 2.183632
H 2.991087 -3.257064 0.890981
H 1.537996 -2.574817 1.676336
H 1.448388 -3.262154 0.017546
H 4.270449 -1.187627 1.210012
H 3.657312 0.419372 0.767602
H 2.916155 -0.491837 2.121697

H 4.000146 -2.071723 -1.128070
H 2.423768 -1.972207 -1.946548
H 3.384093 -0.489682 -1.672809
H 1.273315 0.803338 1.606368
H -1.356853 1.425882 1.209984
H 2.422845 3.145229 -1.157424
H 2.981381 2.357591 0.331730
H 2.683430 1.386610 -1.145203
H 0.775162 4.187726 0.301162
H -0.594198 3.312457 1.001082
H 1.023718 3.190097 1.754140
H 0.132503 3.040150 -1.922176
H 0.244618 1.282928 -2.094035
H -1.096688 2.011048 -1.149790
H -0.418929 -2.194572 -1.760868

51-H$^+$
C 3.280417 -1.727491 -0.172463
C 2.946661 -0.240214 0.038010
C 3.485977 0.590327 -1.146569
C 3.546080 0.254189 1.371406
N 1.457849 -0.092164 0.088940
Si 0.186629 -1.159341 -0.105428
N -1.169479 -0.175351 0.007575
C -2.616594 -0.602730 0.043007
C -3.203873 -0.383095 1.457358
C 0.836953 1.207095 0.478146
C -0.650442 1.270395 -0.028626
C -0.659884 1.789403 -1.483577
C -1.409777 2.226282 0.903783
C -3.453015 0.143924 -1.016048
C -2.669999 -2.113743 -0.272096
H 1.397729 2.035713 0.025737
H 4.637624 0.124932 1.345828
H 3.336147 1.321809 1.534641
H 3.143411 -0.323141 2.217945
H 4.370844 -1.853619 -0.220112
H 2.904087 -2.341531 0.662633
H 2.860485 -2.100566 -1.122260
H 4.579251 0.480793 -1.197816
H 3.052306 0.238673 -2.095239
H 3.262012 1.660846 -1.026952
H -3.718144 -2.442808 -0.268460
H -2.252412 -2.334263 -1.268681
H -2.142844 -2.708783 0.494040
H -4.481392 -0.244721 -0.982598
H -3.498331 1.223061 -0.822561
H -3.050713 -0.023781 -2.025908
H -4.200492 -0.847454 1.501952
H -2.564340 -0.858813 2.216827
H -3.317859 0.679203 1.700329
H 0.882260 1.308905 1.575142
H -0.883920 3.193819 0.901736
H -2.436312 2.405926 0.562032
H -1.430527 1.843889 1.933220
H -0.263656 2.816524 -1.499952

H -0.018897 1.162594 -2.123823
H -1.670556 1.803293 -1.905011
H 0.277835 -2.603167 -0.346284

52-H$^+$
C 1.427135 2.347036 -0.083168
C 0.721866 1.187855 -0.474834
C -0.721839 1.187832 -0.474823
C -1.427162 2.346970 -0.083126
C -0.709273 3.487562 0.262102
C 0.709200 3.487595 0.262080
N 1.270672 -0.027024 -0.874514
C 2.729060 -0.284688 -0.916619
C 3.332678 -0.934147 0.365881
C 2.808150 -2.372024 0.539482
N -1.270627 -0.027049 -0.874485
C -2.729007 -0.284713 -0.916625
C -3.332684 -0.934155 0.365870
C -3.015896 -0.099005 1.621868
Si 0.000030 -1.205353 -0.994382
C 4.861870 -0.978905 0.132734
C 3.015723 -0.099077 1.621890
C -4.861851 -0.979035 0.132598
C -2.808060 -2.371984 0.539579
H -2.514240 2.350226 -0.058571
H -1.246834 4.393491 0.543057
H 1.246723 4.393549 0.543025
H 2.514212 2.350356 -0.058628
H 2.915408 -0.948181 -1.775053
H 3.225696 0.671771 -1.125980
H 5.357895 -1.446394 0.996271
H 5.111739 -1.566509 -0.765402
H 5.270285 0.037217 0.010933
H 3.461499 -0.578197 2.506593
H 3.432220 0.916820 1.541917
H 1.930070 -0.018616 1.792764
H 3.300482 -2.852927 1.398430
H 1.721882 -2.394852 0.753682
H 3.008500 -2.983486 -0.356022
H -2.915339 -0.948218 -1.775053
H -3.225615 0.671758 -1.126001
H -3.461792 -0.578063 2.506546
H -1.930268 -0.018533 1.792884
H -3.432389 0.916886 1.541774
H -5.357915 -1.446504 0.996123
H -5.270324 0.037051 0.010699
H -5.111605 -1.566715 -0.765521
H -3.300474 -2.852913 1.398465
H -3.008243 -2.983489 -0.355937
H -1.721821 -2.394715 0.753926
H 0.000055 -2.150062 -2.129914

53-H$^+$
C 1.040082 3.147916 0.058584
C 1.587675 1.899509 -0.230572
C 0.742479 0.815103 -0.555061

C -0.692473 0.989208 -0.549606
C -1.239498 2.250561 -0.215610
C -0.380670 3.303603 0.061477
N 1.131276 -0.472410 -0.889514
Si -0.274131 -1.511399 -0.929286
N -1.385516 -0.162663 -0.881388
C -2.863822 -0.237983 -0.911238
C -3.540777 -0.733982 0.404277
C -3.217567 -2.219787 0.651553
C 1.921227 4.334759 0.372786
C 2.546078 -0.905905 -0.941397
C 3.110229 -1.537894 0.368344
C 2.942830 -0.588849 1.570964
C 2.420800 -2.884720 0.659066
C 4.612978 -1.787983 0.097080
C -3.102224 0.111417 1.615888
C -5.063194 -0.579742 0.174524
H -2.316736 2.397525 -0.186748
H -0.799876 4.283731 0.295688
H 2.667344 1.767229 -0.213513
H 2.625936 -1.644648 -1.753672
H 3.146655 -0.032797 -1.229101
H 5.080455 -2.248526 0.980172
H 4.755643 -2.466976 -0.759191
H 5.137023 -0.842132 -0.115280
H 3.337024 -1.069966 2.478895
H 3.496266 0.350661 1.418536
H 1.883637 -0.344213 1.749763
H 2.895408 -3.371149 1.525021
H 1.353415 -2.756632 0.919542
H 2.498969 -3.570392 -0.201328
H -3.134952 -0.922041 -1.729913
H -3.238887 0.759530 -1.175454
H -3.587764 -0.269126 2.527321
H -2.011939 0.065783 1.768572
H -3.392997 1.166178 1.494044
H -5.611687 -0.934396 1.059890
H -5.330143 0.475751 0.004238
H -5.396688 -1.170053 -0.694225
H -3.777314 -2.586597 1.525476
H -3.494427 -2.840929 -0.216616
H -2.146320 -2.378941 0.878450
H 2.984146 4.055216 0.397230
H 1.789609 5.127836 -0.382480
H 1.652469 4.771641 1.348880
H -0.391658 -2.417859 -2.094253

54-H$^+$
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N 1.490993 2.267193 -0.112001
C 0.727163 1.236868 -0.486299
C -0.709190 1.239738 -0.474245
C -1.359785 2.405642 -0.029077
C -0.561773 3.490838 0.333861
N 1.281587 0.026595 -0.922055
Si -0.001516 -1.106695 -1.106012

N -1.277874 0.040577 -0.907188
C -2.738988 -0.212477 -0.900329
C -3.273748 -0.930821 0.374115
C -2.717432 -2.364826 0.456662
C 2.744738 -0.220787 -0.883724
C 3.224031 -0.987768 0.384671
C 2.774521 -0.261325 1.667583
C 2.696898 -2.433758 0.376925
C 4.769109 -1.011050 0.301050
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C -4.811115 -0.992625 0.209842
H -2.445345 2.462314 0.024325
H -1.017043 4.423075 0.667974
H 1.479473 4.222334 0.557022
H 3.006506 -0.793803 -1.785828
H 3.227139 0.763028 -0.929979
H 5.182025 -1.558975 1.161235
H 5.109979 -1.510306 -0.620386
H 5.173686 0.013075 0.316720
H 3.181150 -0.778234 2.550012
H 3.127202 0.780208 1.673513
H 1.675233 -0.253043 1.760272
H 3.080008 -2.987386 1.247751
H 1.589144 -2.471107 0.464219
H 2.998574 -2.972562 -0.536390
H -2.969195 -0.824433 -1.785657
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H -3.304936 -0.670171 2.533699
H -1.818357 -0.054618 1.772786
H -3.345570 0.864339 1.634298
H -5.259146 -1.504032 1.074687
H -5.240253 0.020460 0.149883
H -5.093230 -1.546297 -0.700191
H -3.166935 -2.898154 1.307932
H -2.936737 -2.937175 -0.459972
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H -0.026739 -2.146915 -2.147145

55-H$^+$
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C -3.557338 -0.522197 -0.543570
C -2.694332 -1.468988 -1.158767
C 0.701423 0.164075 -0.678499
C 1.590826 -0.938604 -0.682604
C 2.972612 -0.736394 -0.730266
C 3.501350 0.600957 -0.791279
C 2.611851 1.701665 -0.800452
C 1.241481 1.481866 -0.738303
N 4.874533 0.618445 -0.870149
Si 5.629913 -1.032060 -0.934106
N 3.977075 -1.697282 -0.755028
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C 3.643984 -3.735617 0.767134

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N -3.950290 1.538044 0.525329
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C -3.614361 4.088185 0.283319
C -5.021415 4.365502 -0.281473
N -4.914216 -0.596581 -0.421400
C -5.702603 -1.761248 -0.886702
C -5.924980 -2.855155 0.199815
C -6.689665 -2.269403 1.403790
C 5.647387 1.872809 -0.903230
C 6.082965 2.421979 0.488602
C 4.864193 2.769498 1.366549
C 6.970159 1.394804 1.220452
C 6.903343 3.702440 0.212337
C 2.553656 -3.076906 1.636640
C 3.335230 -5.241710 0.607664
Si -5.588509 0.980477 0.092724
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C -6.784632 -3.949258 -0.475753
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H 5.069706 2.640771 -1.441449
H 7.241231 4.148129 1.160709
H 7.793928 3.478067 -0.397260
H 6.296752 4.452465 -0.322232
H 5.205859 3.147003 2.343439
H 4.247380 3.553340 0.897618
H 4.231469 1.886088 1.542019
H 7.357620 1.831006 2.154717
H 6.401785 0.488183 1.486192
H 7.829833 1.095333 0.598676
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H 2.719206 -3.337389 -1.179136
H 2.573862 -3.509546 2.649668
H 2.710995 -1.991291 1.723132
H 1.549570 -3.251165 1.215747
H 3.305165 -5.729472 1.594509
H 2.358387 -5.395318 0.118620
H 4.108648 -5.742013 0.002017
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H 5.821650 -4.004539 0.835764
H 5.251850 -2.505536 1.625018
H -1.183450 1.816284 0.395653
H -3.099306 -2.377820 -1.597194
H -0.680895 -1.964393 -1.648657
H -4.373804 2.964660 1.981002
H -2.646635 2.700523 1.675712
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H -2.821041 3.076692 -1.500664
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H -5.215705 -2.196938 -1.771272
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H -7.756389 -3.545537 -0.803434
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H -6.943952 -3.073543 2.111086
H -6.082881 -1.526414 1.943717
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56-H$^+$
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C 3.725981 -0.716078 -1.455049
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C 4.696319 -2.010787 -3.747271
C 3.316995 -1.982895 -3.488498
P 3.063963 0.145157 0.013554
C 3.337442 1.942744 -0.190874
C 4.136089 2.444674 -1.238068
C 4.347731 3.826236 -1.357371
C 3.768958 4.713645 -0.437227
C 2.968109 4.218696 0.604578
C 2.750841 2.840095 0.730235
C 1.347022 -0.116676 0.220628
Si 0.000014 1.007742 -0.139876
C -1.346986 -0.116654 0.220753
P -3.063937 0.145087 0.013568
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C -5.114848 -0.752906 -1.709959
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C -1.406928 -2.638457 0.701428
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C 0.705216 -3.822689 0.924565
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C -4.822736 -0.117176 3.735224
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C -5.499972 -2.098231 2.501136
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C -3.337527 1.942657 -0.190859
C -4.136205 2.444525 -1.238053
C -4.347955 3.826069 -1.357351

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C -2.968412 4.218625 0.604637
C -2.751035 2.840038 0.730289
C 4.075908 -0.430466 1.437708
C 4.781687 -1.650807 1.383355
C 5.499826 -2.098122 2.501336
C 5.521370 -1.333528 3.677719
C 4.822638 -0.116979 3.735304
C 4.101551 0.334612 2.622078
H 2.496075 -2.656839 0.697063
H 1.252243 -4.751952 1.094832
H -1.252186 -4.751925 1.094984
H -2.496025 -2.656802 0.697366
H -5.814015 -0.289798 -1.011395
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H -5.073306 -2.515628 -4.638470
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H -3.572880 1.285358 2.678193
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H -4.963100 4.206802 -2.174336
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H -2.512256 4.904669 1.320525
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H 4.962853 4.207012 -2.174353
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H 4.840744 0.483919 4.646065
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H 6.667823 -1.420892 -3.057542
H 5.073733 -2.515738 -4.638221
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57-H$^+$
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C -5.745714 -1.097744 3.563922
C -5.072883 -2.112999 2.853043
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C -0.725497 0.855365 1.403179
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C 0.707054 2.403685 3.297738
C -0.703550 2.405013 3.297039
C -1.405927 1.646302 2.361098
C 1.348375 0.044200 0.354966
P 3.053035 0.035428 -0.041217
C 3.297434 -1.209652 -1.358230
C 4.041409 -0.914601 -2.515352
C 4.206734 -1.902997 -3.498093
C 3.634270 -3.171030 -3.333788
C 2.880862 -3.482662 -2.183423
C 2.726199 -2.492184 -1.199803
C 2.236357 -4.844487 -2.019674
C -5.207754 -3.564978 3.264749
C -3.620238 1.661985 -0.647859
C -2.662348 2.661035 -0.889585
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C -4.414192 4.164892 -1.607554
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C -4.207923 -1.893904 -3.499974
C -3.634887 -3.162195 -3.339793
C -2.880372 -3.476900 -2.190975
C -2.725019 -2.489142 -1.204757
C -2.235910 -4.839248 -2.031474
Si 0.000889 -0.573538 -0.649193
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C 4.985299 1.918336 -0.893766
C 5.370135 3.173835 -1.381260
C 4.404584 4.166923 -1.614771
C 3.038913 3.926946 -1.371889
C 2.657307 2.660425 -0.891154
C 1.992750 4.993653 -1.624818
C 4.157472 -0.390959 1.362817
C 4.281445 -1.738838 1.757307
C 5.076581 -2.103129 2.856246
C 5.753171 -1.085961 3.560828
C 5.638856 0.255745 3.175973
C 4.843678 0.611416 2.076464
C 5.209310 -3.553451 3.274426
H -2.495074 1.655984 2.374759
H -1.250531 3.001186 4.030124
H 1.254422 2.998807 4.031378
H 2.498133 1.651406 2.377186
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H 4.716661 5.147154 -1.982539
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H 6.171225 1.030781 3.730108
H 4.762733 1.656851 1.778501
H 4.474495 0.074998 -2.657577

H 4.781056 -1.676943 -4.398139
H 3.769290 -3.931017 -4.107116
H 2.136006 -2.718403 -0.309925
H -4.475754 0.081570 -2.653459
H -4.783082 -1.665467 -4.398881
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H 6.264903 -3.871691 3.268538
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H -6.264166 -3.880498 3.261396
H -1.817004 -4.968790 -1.021904
H -2.963643 -5.647144 -2.210161
H -1.416633 -4.973782 -2.758941
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H -1.318447 4.704418 -2.425000
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58-H$^+$
C 1.694153 -3.144716 -0.253442
Si 2.533923 -1.544131 0.327991
C 2.590132 -1.571624 2.230375
C 1.452931 0.004968 -0.253407
Si 2.582447 1.630716 -0.227713
C 3.721341 1.594829 -1.744091
Si -0.011077 0.130058 0.819180
C -1.477764 0.139909 -0.254186
Si -2.766581 1.505409 0.323752
C -3.550018 0.949836 1.963645
C 0.704804 -0.143562 -1.655257
C -0.738894 0.465384 -1.622605
Si -2.348920 -1.642995 -0.255646
C -1.654610 -2.687370 -1.681912
C 1.501643 3.184992 -0.373153
C 3.551287 1.730256 1.399582
C 4.286398 -1.511718 -0.391044
C -2.019347 -2.458182 1.435975
C -4.217174 -1.548611 -0.579624
C -1.840433 3.130641 0.670821

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H 1.282359 0.337704 -2.458146
H -1.314676 0.083885 -2.478734
H -0.667629 1.558544 -1.744164
H 3.309041 -2.342648 2.556290
H 2.911427 -0.617137 2.673277
H 1.616484 -1.840840 2.676694
H 4.800716 -2.435273 -0.073024
H 4.278628 -1.503039 -1.492730
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H 2.299897 -4.000121 0.091820
H 0.682306 -3.273676 0.162409
H 1.625885 -3.220649 -1.350613
H 4.317818 2.523936 -1.741236
H 4.421324 0.748703 -1.761982
H 3.148881 1.586309 -2.686096
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H 2.886145 1.747719 2.279444
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H 2.159675 4.060963 -0.507693
H 0.826006 3.154134 -1.243024
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H -4.610629 -2.578053 -0.507790
H -4.791166 -0.926563 0.120433
H -4.422894 -1.193138 -1.601924
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H -2.246662 -3.617118 -1.739510
H -1.772885 -2.174002 -2.650192
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59-H$^+$
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C -4.255369 -0.684092 -0.208566
C -5.526150 -1.295676 -0.169984
C -6.685081 -0.516449 -0.029212
C -6.588324 0.881819 0.073234
Si -2.613449 -1.587152 -0.415797
C -2.456528 -3.113748 0.692655
Si -2.418522 1.437418 -0.228301
C -2.021065 2.060174 -1.983238
C -1.365524 -0.194910 0.158226
Si 0.250153 -0.074391 -0.640497

C 1.431312 0.234801 0.697410
Si 2.735475 1.630726 0.313238
C 3.229562 2.433495 1.956443
C 0.432115 0.487150 1.894061
C -0.909546 -0.277433 1.674725
Si 2.567370 -1.364013 0.840610
C 1.722046 -2.925773 0.142998
C 4.022619 -0.808191 -0.218595
C 4.101666 0.594906 -0.470537
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C 6.138876 0.232445 -1.769551
C 6.060758 -1.148504 -1.520823
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C 1.999836 2.923755 -0.871955
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H 3.715893 -2.418216 2.790550
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H 6.957088 0.631140 -2.372443
H 6.817793 -1.819467 -1.931322
H 4.957093 -2.744553 -0.572061
H -1.002303 2.479928 -2.068189
H -2.133059 1.266766 -2.740468
H -2.721290 2.867318 -2.257956
H -1.050213 3.238444 0.893675
H -2.783042 3.621474 0.907277
H -2.137195 2.447668 2.072019
H -1.311362 -2.545935 -2.370907
H -3.063832 -2.703646 -2.611785
H -2.283310 -1.134366 -2.878078
H -1.463027 -3.586362 0.615197
H -2.646344 -2.874308 1.750891
H -3.199893 -3.870088 0.387473
H -5.272539 2.594450 0.118945
H -7.491967 1.483476 0.188544
H -7.664342 -0.997785 0.006079
H -5.619474 -2.382858 -0.242160
H 0.557641 -0.202874 -2.087124

60-H$^+$

N 2.412943 0.568097 1.290828
C 2.361449 0.974179 -0.008141
N 3.601014 1.466187 -0.287241
C 4.432729 1.358682 0.824037
C 3.677794 0.785721 1.825489
Si 0.858402 0.687104 -1.164581
C -0.756421 1.397870 -0.551878
C -1.101929 2.828380 -0.592358
C -2.358746 3.303404 -1.042179
C -2.620630 4.676127 -1.102588
C -1.642552 5.608316 -0.713394
C -0.388508 5.155754 -0.273810
C -0.121156 3.781917 -0.223097
C 4.048677 2.024319 -1.571444
C 5.857469 1.814999 0.815182
C 4.044021 0.427421 3.231271
C 1.294029 -0.057804 2.015753
C 0.356563 -1.095235 -0.926096
C 1.317139 -2.210771 -0.930314
C 1.293606 -3.248336 0.037001
C 2.288847 -4.232235 0.055817
C 3.329340 -4.214176 -0.889462
C 3.370594 -3.193962 -1.853187
C 2.382027 -2.201643 -1.865865
C -0.946002 -1.059720 -0.468157
C -1.705862 -2.281302 -0.106195
C -2.346259 -2.401699 1.146807
C -3.015693 -3.583728 1.490236
C -3.071761 -4.652020 0.580415
C -2.450180 -4.535494 -0.674645
C -1.766970 -3.361880 -1.013270
C -1.572393 0.306753 -0.309914
C -2.988815 0.429788 0.116680
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C -4.656914 1.373923 1.627894
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C -5.350679 -0.112962 -0.166760
C -4.015580 -0.255718 -0.567228
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H -3.502182 -3.666562 2.463872
H -3.603430 -5.567963 0.844645
H -2.499012 -5.359149 -1.389171
H -1.274923 -3.269065 -1.982572
H -2.532560 1.781226 1.745379
H -4.903002 2.001954 2.486110
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H -6.136972 -0.640896 -0.709142
H -3.762817 -0.897756 -1.411691
H -3.119591 2.590419 -1.356279
H -3.591965 5.022186 -1.460814
H -1.854693 6.677901 -0.759485
H 0.378672 5.871953 0.027516
H 0.854307 3.432278 0.129595
H 0.489247 -3.279104 0.771328
H 2.250854 -5.020236 0.810694
H 4.097919 -4.988949 -0.875734

H 4.169034 -3.174597 -2.597749
H 2.409549 -1.420036 -2.630919
H 6.328415 1.587662 1.780327
H 6.436947 1.310350 0.024934
H 5.935314 2.902225 0.647152
H 3.890308 -0.646636 3.424261
H 5.102211 0.658240 3.410197
H 3.445260 0.993351 3.964197
H 1.427794 0.128323 3.087366
H 0.354288 0.395226 1.677244
H 1.284637 -1.137139 1.811699
H 4.766083 1.336613 -2.041715
H 3.184472 2.164373 -2.226709
H 4.533331 2.992542 -1.389672
H 1.294814 1.167736 -2.499518

61-H$^+$
C -4.282699 0.444138 -0.881169
C -3.170555 0.912490 -0.150362
C -3.385761 1.763813 0.955487
C -4.683973 2.137507 1.322240
C -5.785205 1.675824 0.581039
C -5.580566 0.832653 -0.522970
C -1.788675 0.512900 -0.515812
C -1.439060 -0.954288 -0.631584
C -2.444494 -1.997094 -0.310130
C -3.149419 -1.979586 0.913566
C -4.049276 -3.006301 1.228424
C -4.271866 -4.052020 0.317666
C -3.585560 -4.069940 -0.908344
C -2.673239 -3.053825 -1.217373
C -0.139772 -1.254290 -0.993842
C 0.584837 -2.533761 -0.937264
C 0.293906 -3.541999 0.016642
C 1.086143 -4.692528 0.105081
C 2.182554 -4.874550 -0.756172
C 2.485486 -3.887814 -1.707975
C 1.700657 -2.730230 -1.789693
Si 0.724591 0.389289 -1.194360
C -0.756793 1.415176 -0.700702
C -0.794846 2.885013 -0.737333
C -1.915478 3.619594 -1.198750
C -1.882400 5.017304 -1.243694
C -0.737622 5.720482 -0.828287
C 0.386688 5.010270 -0.379160
C 0.358901 3.610236 -0.343802
C 2.185738 0.411804 0.059194
N 2.047859 0.261151 1.408393
C 3.294508 0.297230 2.021892
C 4.228676 0.467935 1.019080
N 3.524426 0.526831 -0.180922
C 0.722547 0.096031 2.088887
C 0.673228 -1.184165 2.936403
C 4.114072 0.711367 -1.545697
C 4.537012 2.174112 -1.751180
C 5.719930 0.541309 1.156804

C 3.539448 0.126493 3.490955
C 5.219640 -0.315150 -1.842817
C 0.326615 1.376001 2.839950
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H -4.583815 -2.984616 2.179953
H -4.981308 -4.845629 0.559269
H -3.761109 -4.876216 -1.622784
H -2.128625 -3.068634 -2.162643
H -2.526641 2.133727 1.517642
H -4.838047 2.789954 2.183877
H -6.797418 1.969510 0.864917
H -6.432211 0.469847 -1.101132
H -4.125580 -0.226021 -1.727233
H -2.803791 3.086639 -1.534083
H -2.753605 5.562940 -1.611039
H -0.720409 6.811141 -0.863206
H 1.283500 5.545636 -0.060569
H 1.237360 3.062899 0.011563
H -0.549990 -3.412143 0.692447
H 0.846059 -5.453404 0.850512
H 2.791746 -5.777478 -0.686840
H 3.326780 -4.023503 -2.390966
H 1.930821 -1.975083 -2.547303
H 5.980658 0.750102 2.202753
H 6.200354 -0.408922 0.875381
H 6.155363 1.336564 0.537216
H 3.481092 -0.932857 3.787196
H 4.544803 0.489642 3.742302
H 2.817370 0.686249 4.098656
H 0.009603 -0.038536 1.274723
H 3.290501 0.498497 -2.232543
H -0.698004 1.247192 3.220250
H 0.981908 1.581622 3.698014
H 0.336801 2.241280 2.161446
H -0.380593 -1.382088 3.183426
H 1.056775 -2.042143 2.365011
H 1.228125 -1.088838 3.878811
H 4.886773 2.302045 -2.786438
H 3.684683 2.850323 -1.584669
H 5.355131 2.463456 -1.076569
H 5.402856 -0.309323 -2.927548
H 6.166019 -0.071911 -1.344203
H 4.901251 -1.327000 -1.550281
H 1.287843 0.763025 -2.514350

62-H$^+$
C 5.514759 1.725475 0.163483
C 4.774322 0.642641 0.639887
C 3.409420 0.612714 0.304859
C 2.803413 1.659678 -0.421149
C 3.557861 2.730992 -0.931039
C 4.920084 2.741926 -0.628110
N 1.447912 1.351065 -0.512304
C 1.213478 0.138675 0.073978
N 2.404862 -0.314935 0.572793
Si -0.500432 -0.801213 0.152693

N -1.433670 -0.484782 -1.268867
C -1.071158 -0.784985 -2.661861
C -1.665634 -2.097672 -3.243561
C -1.214824 -3.302571 -2.394473
C 2.638488 -1.612085 1.247978
C 3.183785 -2.761520 0.344682
C 4.651406 -2.517051 -0.064711
C 0.420949 2.270649 -1.062221
C 0.007903 3.463596 -0.139479
C 1.057124 4.595429 -0.137524
C -2.561407 0.309365 -0.917679
C -2.681730 0.521260 0.488287
C -3.711643 1.324704 0.989890
C -4.621456 1.922090 0.097067
C -4.498036 1.721155 -1.283028
C -3.465426 0.913548 -1.797449
N -1.652514 -0.106493 1.236907
C -1.538418 0.002674 2.699448
C -2.196768 -1.148379 3.505120
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C -3.206152 -2.043768 -3.281333
C -1.113785 -2.242600 -4.678596
C 3.108211 -4.037799 1.216278
C 2.329226 -2.950999 -0.924192
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C -0.237968 3.002646 1.308910
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H -5.205618 2.184621 -1.971618
H -5.427874 2.541213 0.492135
H -3.817165 1.477103 2.062704
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H -1.960984 0.968733 3.017118
H -2.390495 -1.639550 5.624892
H -0.852854 -0.832322 5.215337
H -2.369285 0.112237 5.293371
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H -4.207716 -0.279334 3.575826
H -3.926798 -1.342907 2.170118
H -1.943147 -3.301329 3.764768
H -1.777474 -2.760976 2.076812
H -0.456273 -2.462974 3.251788
H 0.030522 -0.853295 -2.714536
H -1.366174 0.068404 -3.295194
H -3.602828 -2.996431 -3.666118
H -3.624443 -1.873488 -2.278426
H -3.558315 -1.238567 -3.945573
H -1.505764 -3.159414 -5.145308
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H 5.236131 -0.148599 1.225300
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H 3.099917 3.519825 -1.522074
H 3.352063 -1.415544 2.061388
H 1.689381 -1.913477 1.705945
H 0.817592 2.654038 -2.014028
H -0.457440 1.658587 -1.281090
H 2.785932 -3.724822 -1.559867
H 1.310542 -3.279833 -0.679329
H 2.272401 -2.023597 -1.518283
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H 2.067302 -4.262419 1.500329
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H 0.642717 5.468587 0.389308
H 1.980819 4.301780 0.381794
H 1.307828 4.912080 -1.163817
H -0.502010 3.875381 1.925507
H -1.066293 2.288129 1.357180
H 0.663797 2.543257 1.746582
H -1.649358 4.876343 -0.166605
H -1.164332 4.324911 -1.789292
H -2.103971 3.239750 -0.719131
H -0.087551 -2.178668 0.459854

63-H$^+$
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C 1.209066 0.051999 1.088965
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C -0.794003 -0.093091 2.300713
C -0.471316 -1.554129 2.801948
C 1.078046 -1.519497 3.042573
N -0.818771 -0.045048 -0.282513
Si 0.236481 0.066779 -1.695399
P 2.148680 0.046751 -0.409311
C 3.134803 -1.555958 -0.600285
C 2.093223 -2.702992 -0.625606
C -2.259098 0.095104 -0.373747
C -3.038642 -1.062792 -0.605191
C -4.430887 -0.899198 -0.722749
C -5.023254 0.363291 -0.600286
C -4.229258 1.490957 -0.356577
C -2.831903 1.384078 -0.243248
C -2.425025 -2.455905 -0.720134
C -2.609601 -3.027390 -2.145399
C -1.995636 2.636019 0.015248
C -2.154920 3.661574 -1.131038
C 3.118526 1.652429 -0.674314
C 4.448229 1.633164 0.113878
C 3.392478 1.864588 -2.181582
C 2.217331 2.795770 -0.147191
C -2.355186 3.276999 1.376083
C -3.017965 -3.419370 0.334056
C 3.958600 -1.558483 -1.904747

C 4.060966 -1.740247 0.626408
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H 3.920914 2.823927 -2.301789
H 4.025282 1.075794 -2.608666
H 2.458109 1.926308 -2.761176
H 4.903271 2.634094 0.040995
H 4.294827 1.408777 1.180645
H 5.162029 0.911055 -0.307088
H 2.751897 3.747059 -0.300575
H 1.261832 2.856479 -0.691860
H 2.001288 2.679855 0.924390
H -4.695862 2.472282 -0.257152
H -6.105751 0.468654 -0.691332
H -5.054604 -1.775674 -0.905458
H -0.934260 2.351208 0.060995
H -1.723485 4.161515 1.556877
H -3.407329 3.601469 1.389021
H -2.207246 2.565775 2.203539
H -1.512843 4.538223 -0.947526
H -1.881060 3.220416 -2.102795
H -3.196402 4.012201 -1.200246
H -1.344569 -2.376596 -0.524094
H -2.138114 -4.020304 -2.222547
H -3.679372 -3.137808 -2.382974
H -2.161938 -2.365362 -2.904337
H -2.525304 -4.402491 0.266691
H -2.883638 -3.026005 1.353816
H -4.095886 -3.568867 0.167115
H 4.545676 -2.726005 0.539262
H 4.849754 -0.979152 0.670636
H 3.495895 -1.721801 1.568487
H 4.420763 -2.551958 -2.020239
H 3.331220 -1.374370 -2.791587
H 4.766340 -0.813868 -1.876311
H 2.636166 -3.661219 -0.600622
H 1.423201 -2.665001 0.246936
H 1.486091 -2.686160 -1.543020
H 2.456000 0.271779 2.942843
H -1.850743 0.188839 2.354513
H -1.018606 -1.741808 3.736786
H -0.777798 -2.313924 2.069361
H 1.608607 -2.290191 2.467034
H 1.316584 -1.665617 4.106679
H 0.087787 0.619546 4.212895
H 0.257065 1.793468 2.853640
H 0.083577 1.349400 -2.422282

64-H$^+$
C 0.357449 3.555814 -0.244270
C 0.822195 2.345670 -0.805627
C 2.148202 2.296517 -1.310822
C 2.981067 3.421218 -1.236922
C 2.504532 4.613667 -0.669251
C 1.191854 4.680811 -0.176771
Si -0.110234 0.744358 -0.964240
P -2.261640 0.271938 -0.240949

C -2.989306 1.423083 1.067361
C -1.850537 1.662871 2.091862
C -1.729108 -1.254188 0.476344
C -0.358144 -1.454535 0.508812
C -0.093056 -2.739608 1.265193
C -0.430755 -2.425357 2.773278
C -1.989216 -2.260689 2.769561
C -2.354714 -2.424087 1.249960
C -1.354545 -3.552080 0.850670
N 0.572238 -0.570525 0.026490
C 1.990351 -0.853847 -0.004900
C 2.819312 -0.293121 0.996384
C 4.207503 -0.489465 0.880928
C 4.750617 -1.221859 -0.181314
C 3.906741 -1.790629 -1.143278
C 2.512020 -1.619627 -1.076787
C 2.263535 0.461088 2.202217
C 2.792320 1.910853 2.282568
C 1.622118 -2.276710 -2.131215
C 1.960807 -1.773292 -3.552859
C -3.344912 0.025102 -1.778434
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C -2.815160 -1.232550 -2.508381
C 1.731548 -3.817924 -2.057343
C 2.601631 -0.300727 3.507105
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C -4.167783 0.731736 1.796504
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H -3.573624 2.180522 -2.221002
H -2.183183 1.408079 -3.044056
H -5.381722 -0.463884 -2.298912
H -4.939735 -1.023288 -0.667281
H -5.277896 0.710204 -0.969241
H -3.416768 -1.372149 -3.421176
H -1.762428 -1.126030 -2.808105
H -2.909748 -2.131002 -1.881793
H 4.330668 -2.378740 -1.959059
H 5.831019 -1.359775 -0.253665
H 4.866443 -0.064232 1.639654
H 0.573624 -2.015526 -1.926412
H 1.066155 -4.281230 -2.803398
H 2.761618 -4.146692 -2.266114
H 1.451000 -4.189030 -1.059101
H 1.286843 -2.237600 -4.290538
H 1.856556 -0.678739 -3.625775
H 2.994920 -2.035292 -3.826367
H 1.168067 0.505770 2.107079
H 2.373774 2.411581 3.170627
H 3.889795 1.918137 2.378045
H 2.520682 2.489638 1.390253
H 2.122083 0.190252 4.369224
H 2.264626 -1.347512 3.462839
H 3.689183 -0.304198 3.680467
H -4.466959 1.375201 2.639909
H -5.042182 0.600305 1.147840

H -3.877630 -0.245911 2.203927
H -3.736024 3.444040 1.261210
H -2.693213 3.237637 -0.168730
H -4.361446 2.607939 -0.177085
H -2.240202 2.304952 2.898115
H -1.515389 0.715056 2.538234
H -0.978390 2.164890 1.649330
H -3.416822 -2.617734 1.052406
H 0.893151 -3.186361 1.097647
H -0.115690 -3.272710 3.398983
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H -2.305330 -1.291640 3.178160
H -2.473474 -3.052350 3.360886
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H -1.379287 -3.791624 -0.222553
H 2.546446 1.376157 -1.745575
H 4.001002 3.363743 -1.620518
H 3.153546 5.489233 -0.613146
H 0.816568 5.608131 0.259355
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H -0.122264 0.312448 -2.383964

65-H$^+$

C	0.041819	-1.062205	3.471385
C	0.483007	0.291901	2.819027
C	0.374417	0.136544	1.299262
C	-0.988199	0.084777	1.003052
C	-1.742200	0.195205	2.309657
C	-1.471003	-1.164310	3.067224
C	-0.788062	1.155492	3.079904
N	-1.525116	-0.088030	-0.242590
Si	-0.309221	-0.084441	-1.543567
P	1.458072	0.002535	-0.049659
Si	3.995288	-0.107879	-0.399090
C	4.752622	-0.142468	-2.122995
C	-2.945489	0.068920	-0.485694
C	-3.485689	1.375677	-0.564790
C	-4.862573	1.496729	-0.822794
C	-5.666614	0.363974	-1.001824
C	-5.105779	-0.915930	-0.917215
C	-3.735102	-1.092126	-0.653490
C	-2.638078	2.632798	-0.377681
C	-2.655169	3.515305	-1.646885
C	-3.154576	-2.499918	-0.547768
C	-3.254855	-3.244418	-1.898989
N	2.713802	1.123629	-0.167371
C	2.661275	2.603756	-0.326796
C	1.544678	3.203833	0.551349
N	2.619508	-1.227018	-0.140292
C	2.442377	-2.690113	-0.360224
C	2.492527	-3.004541	-1.871739
C	-3.845730	-3.306224	0.576000
C	-3.100895	3.441077	0.856645
C	5.303313	-0.144640	0.950645
C	3.604959	-3.400655	0.362634
C	1.100787	-3.169491	0.230088

C	4.027332	3.156234	0.128503
C	2.418573	2.960409	-1.809659
H	-0.342732	-1.333974	-2.337432
H	-5.305014	2.492454	-0.885962
H	-6.732774	0.479668	-1.204744
H	-5.737374	-1.795640	-1.051549
H	-1.594345	2.334919	-0.197659
H	-2.455784	4.323790	0.993685
H	-4.136327	3.792113	0.726202
H	-3.059906	2.830930	1.772083
H	-2.009080	4.396371	-1.503392
H	-2.298992	2.955673	-2.526378
H	-3.674662	3.871575	-1.861251
H	-2.088526	-2.417603	-0.286512
H	-2.806034	-4.247306	-1.815895
H	-4.307604	-3.365068	-2.199176
H	-2.736088	-2.691550	-2.698683
H	-3.388612	-4.305050	0.660761
H	-3.755481	-2.793365	1.546505
H	-4.917346	-3.440046	0.360908
H	1.438038	0.691332	3.182542
H	-2.798133	0.469520	2.217895
H	-2.123560	-1.215711	3.950525
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H	2.369830	-4.085696	-2.040890
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66-H$^+$

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C	-1.049889	5.258265	-1.420993
C	-0.010021	1.893129	0.082384
C	-0.782532	0.669952	-0.648519
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C	-1.828572	0.736481	-2.974850
C	-2.884209	1.078758	-3.832859
C	-4.020055	1.729251	-3.325206
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C	-3.030856	1.699931	-1.104670
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C	4.224793	-1.026607	-1.140161
C	5.589780	-0.809842	-1.397771
C	6.249583	0.320470	-0.899551
C	5.557941	1.242124	-0.106777
C	4.192708	1.068287	0.188854
C	3.522296	-2.258459	-1.704939
C	4.334740	-3.555552	-1.498298
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C	0.295048	-1.284585	1.189505
C	0.377527	-2.205647	2.420993
C	0.865719	-1.334484	3.632268
C	2.323013	-0.946109	3.207260
C	2.512499	-1.708249	1.842681
C	1.680746	-2.989287	2.102778
P	-1.180052	-0.793077	0.373450
N	-2.585469	-0.688450	1.302485
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C	-1.384122	-3.025305	-1.449615
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H	1.572540	1.286028	-2.382350

67-H$^+$

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68-H$^+$
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69-H$^+$
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C 1.725261 -2.292589 2.737171
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H 0.689558 -2.548750 -3.108531
H 1.768264 -3.967833 -3.169544
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70-H$^+$
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72-H$^+$

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73-H$^+$
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74-H$^+$
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C -4.763964 2.278283 -0.846551
C -3.751334 2.639062 0.053391
C -2.807824 1.700570 0.509484
C -4.038642 -1.435975 -1.457197
C -3.600713 -1.443441 -2.942142
C -1.694934 2.101803 1.484704
C -1.288381 3.585081 1.358364
C -2.234743 -1.442892 1.538533
C -3.619710 -1.432529 2.131778
C -1.249891 -2.295170 2.072953
C 0.118114 -2.288098 1.733906
C 1.103238 -3.060888 2.570203
N 0.589657 -1.573782 0.681361
C 2.015800 -1.370069 0.466766
C 2.678723 -0.369281 1.219326
C 4.044299 -0.163561 0.956033
C 4.720822 -0.910393 -0.015214
C 4.037295 -1.885938 -0.749641
C 2.672030 -2.144003 -0.521925
C 1.983153 0.490562 2.273237
C 1.950186 1.972901 1.834926
C 1.969996 -3.236242 -1.328759
C 1.911938 -2.862381 -2.829202
C 2.660532 -4.607095 -1.136083
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H 4.565645 -2.470108 -1.504233
H 5.780354 -0.728564 -0.203048
H 4.576427 0.606454 1.515272
H 0.936670 -3.339511 -0.965590
H 2.111057 -5.383889 -1.690093
H 3.693894 -4.584798 -1.514661
H 2.693248 -4.892752 -0.072648
H 1.396065 -3.652632 -3.396539
H 1.375642 -1.913963 -2.997456
H 2.928037 -2.753846 -3.239988
H 0.941411 0.153413 2.382352
H 2.110985 0.939807 4.403548
H 2.731717 -0.684202 3.995639
H 3.697341 0.760059 3.616214
H 1.475575 2.579113 2.622902
H 2.969287 2.356283 1.673466

H 1.390269 2.098819 0.900014
H -3.689336 3.669976 0.399631
H -5.479873 3.028856 -1.185684
H -5.631507 0.693973 -2.032000
H -3.347652 -2.089473 -0.902780
H -3.630788 -2.469209 -3.342541
H -4.276758 -0.817193 -3.545212
H -2.577544 -1.052188 -3.062584
H -5.465535 -3.071286 -1.669122
H -5.798861 -2.018464 -0.263279
H -6.188276 -1.463474 -1.908683
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H -1.286398 2.148157 3.626626
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H -2.202583 0.710032 3.123063
H -0.388234 3.766580 1.962216
H -1.062272 3.855058 0.316030
H -2.080600 4.254480 1.729002
H -3.650916 -2.013412 3.061707
H -3.959168 -0.405522 2.326008
H -4.326839 -1.869195 1.407902
H -1.549452 -2.938247 2.896713
H 1.783519 -3.637390 1.924930
H 1.728789 -2.368203 3.153642
H -0.735351 1.265971 -1.413892
H 1.756280 -0.016968 -1.831641
H 3.815487 0.932864 -1.920051
H 5.191608 2.992123 -1.666673
H 4.084028 5.208503 -1.304256
H 1.586232 5.342056 -1.247378
H 0.214293 3.299854 -1.551520
H -0.776139 -1.873306 -1.555399

75-H$^+$
C 3.477546 -1.082598 -0.391986
C 2.664907 0.037236 -0.090933
C 3.050448 1.367557 -0.391220
C 4.301147 1.556946 -1.005127
C 5.130085 0.471279 -1.310336
C 4.717832 -0.831017 -1.007559
N 1.363675 -0.169495 0.546041
Si 0.000033 -0.313782 -0.577659
O -0.001196 -1.790935 -1.308278
C 2.180703 2.584093 -0.075434
C 1.841772 3.373114 -1.361442
C 3.074237 -2.524424 -0.087916
C 2.954750 -3.342870 -1.395488
C 1.249727 -0.185773 1.901067
C 2.507326 -0.102589 2.724125
C -0.000018 -0.240127 2.539586
C -1.249686 -0.185802 1.900914
C -2.507344 -0.102657 2.723886
N -1.363635 -0.169580 0.545865
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C -3.478015 -1.081815 -0.391990
C -4.718163 -0.829682 -1.007610

C -5.129775 0.472778 -1.310547
C -4.300355 1.558079 -1.005352
C -3.049794 1.368140 -0.391337
C -3.075462 -2.523796 -0.087690
C -2.955959 -3.342380 -1.395170
C -2.179597 2.584327 -0.075449
C -1.840330 3.373375 -1.361344
C -2.865606 3.511305 0.956121
C -4.085297 -3.210159 0.863672
C 2.867001 3.510954 0.956040
C 4.083464 -3.211367 0.863666
H -2.275506 -0.150089 3.794925
H -4.623176 2.572502 -1.243484
H -6.097546 0.642686 -1.785386
H -5.365675 -1.673413 -1.249022
H -1.231458 2.244217 0.368936
H -2.210949 4.365850 1.189013
H -3.812169 3.904802 0.554662
H -3.089652 2.980804 1.895003
H -1.188655 4.226821 -1.119193
H -1.324140 2.737792 -2.097127
H -2.754899 3.766266 -1.831393
H -2.089539 -2.524814 0.398558
H -3.750116 -4.235372 1.085358
H -4.194721 -2.670285 1.817290
H -5.080685 -3.271774 0.397116
H -2.608185 -4.362297 -1.168763
H -3.933062 -3.416274 -1.897937
H -2.243882 -2.875648 -2.090615
H 5.364954 -1.675029 -1.249031
H 6.097976 0.640775 -1.785076
H 4.624453 2.571232 -1.243189
H 1.232426 2.244339 0.368923
H 1.190410 4.226833 -1.119421
H 2.756505 3.765596 -1.831508
H 1.325358 2.737632 -2.097156
H 2.212645 4.365780 1.188745
H 3.090776 2.980533 1.895031
H 3.813738 3.904033 0.554579
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H 3.747858 -4.236519 1.084995
H 5.079022 -3.273178 0.397504
H 4.192625 -2.671740 1.817449
H 2.605928 -4.362484 -1.169368
H 2.243530 -2.875542 -2.091457
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H 2.275394 -0.149755 3.795155
H 3.193907 -0.919325 2.458348
H 3.039808 0.836442 2.506869
H -0.000096 -0.263435 3.626400
H -3.039685 0.836500 2.506810
H -3.193996 -0.919242 2.457851
H 0.004108 -1.822229 -2.278471
H 0.000822 0.774952 -1.566646

76-H$^+$

C 3.292951 -0.719425 0.938998
C 2.828243 0.383136 0.178230
C 3.434229 0.797783 -1.031384
C 4.534378 0.050967 -1.489615
C 5.008351 -1.053103 -0.773108
C 4.397415 -1.425431 0.430686
N 1.615107 1.071078 0.622030
Si 0.142580 0.536667 -0.189522
O 0.007456 -1.141062 -0.140131
S 0.196396 -2.192735 -1.432752
O 0.968378 -1.527942 -2.485216
C 2.971091 2.018916 -1.824096
C 2.553669 1.638193 -3.263889
C 2.671783 -1.155133 2.267141
C 2.123919 -2.600115 2.194968
C 1.637463 2.037304 1.578819
C 2.977073 2.509263 2.071368
C 0.455659 2.593508 2.099527
C -0.850933 2.180948 1.791079
C -2.026487 2.807076 2.489138
N -1.101579 1.227888 0.850536
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C -2.892424 -0.407662 1.331715
C -4.159105 -0.923614 1.005936
C -4.941158 -0.349581 -0.003876
C -4.476426 0.769395 -0.703751
C -3.220544 1.334697 -0.418386
C -2.088738 -1.040706 2.469111
C -1.866999 -2.557533 2.265613
C -2.754025 2.568599 -1.190583
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C -3.742100 3.745316 -1.002677
C -2.796623 -0.806111 3.827452
C -1.637473 -2.258009 -1.992689
F -1.690843 -2.969456 -3.116883
O 0.549553 -3.486261 -0.861453
F -2.377111 -2.822985 -1.038917
F -2.058352 -1.000570 -2.216872
C 4.077181 3.101470 -1.853360
C 3.700625 -1.057254 3.421102
H -1.694078 3.503076 3.268892
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H -5.918673 -0.772786 -0.241376
H -4.531789 -1.789102 1.554925
H -1.777475 2.889126 -0.794448
H -3.357221 4.644079 -1.508878
H -4.722956 3.501992 -1.439221
H -3.897790 3.982468 0.061727
H -2.242647 3.169468 -3.226193
H -1.837276 1.466956 -2.867611
H -3.531063 1.941177 -3.140720
H -1.098866 -0.562228 2.516021
H -2.193972 -1.236247 4.642670
H -2.951582 0.262827 4.040569
H -3.781945 -1.297330 3.834507
H -1.278543 -2.956172 3.106512

H -2.828449 -3.093936 2.244812
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H 4.775384 -2.282017 0.989967
H 5.859135 -1.622697 -1.150480
H 5.020151 0.346659 -2.420191
H 2.095338 2.460835 -1.322571
H 2.180827 2.529397 -3.793050
H 3.416386 1.247128 -3.825140
H 1.772340 0.864509 -3.267448
H 3.718785 3.992063 -2.393062
H 4.375916 3.405242 -0.837156
H 4.972878 2.724289 -2.370726
H 1.828236 -0.488715 2.505146
H 3.216460 -1.317666 4.375203
H 4.528205 -1.764193 3.256001
H 4.137253 -0.050975 3.518041
H 1.668975 -2.871473 3.160969
H 1.372043 -2.710699 1.405504
H 2.939830 -3.311529 1.993417
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H 3.523983 1.682783 2.546987
H 3.591191 2.842176 1.219782
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H -2.644604 3.349232 1.755704
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77-H$^+$
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C -2.663694 0.052133 -0.015483
C -3.581949 -0.994942 -0.251776
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C -5.109832 0.672677 -1.171938
C -4.169621 1.685412 -0.939406
N -1.383600 -0.261541 0.612970
Si -0.028177 -0.747535 -0.445726
S 0.007586 0.296925 -2.295285
C -3.272115 -2.455056 0.073174
C -3.035995 -3.253389 -1.231693
C -1.887767 2.510561 -0.145718
C -1.883367 3.552127 -1.285322
C -1.274798 -0.289451 1.968719
C -2.530778 -0.172535 2.793289
C -0.033038 -0.440414 2.611444
C 1.222320 -0.392434 1.982173
C 2.475683 -0.361935 2.817039
N 1.349994 -0.363554 0.626910
C 2.646868 -0.082799 0.017011
C 3.033903 1.269545 -0.143865
C 4.273661 1.514014 -0.760288
C 5.085989 0.462775 -1.202514
C 4.675266 -0.862957 -1.025540
C 3.449064 -1.166512 -0.406348
C 2.178966 2.450676 0.318012
C 1.818856 3.379912 -0.864645
C 3.038869 -2.625359 -0.213869

C 2.773684 -3.304846 -1.577909
C 4.101304 -3.413712 0.587009
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H 2.233811 -0.446577 3.883709
H 5.313978 -1.679770 -1.364931
H 6.041932 0.677960 -1.682823
H 4.600512 2.545499 -0.898683
H 2.103207 -2.659205 0.365485
H 3.757158 -4.446399 0.752908
H 5.055244 -3.456726 0.039428
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H 2.441637 -4.344302 -1.427948
H 1.999329 -2.768618 -2.150463
H 3.690640 -3.320718 -2.187393
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H 2.248115 4.095461 1.752917
H 3.145722 2.654118 2.298206
H 3.830231 3.702080 1.033119
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H 2.727503 3.820591 -1.302938
H 1.286618 2.839016 -1.659815
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H -5.541657 -1.439671 -1.042636
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H -3.946755 -3.257695 -1.850698
H -2.223537 -2.811769 -1.831038
H -4.094148 -4.147314 1.176839
H -4.585467 -2.562981 1.842586
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H -1.035123 4.239201 -1.151550
H -1.792508 3.066148 -2.268092
H -2.803231 4.156954 -1.279337
H -2.289294 -0.100368 3.860890
H -3.126354 0.699425 2.488457
H -3.161579 -1.059522 2.621861
H -0.041175 -0.496803 3.696975
H 3.141814 -1.187164 2.519484
H 3.035906 0.568210 2.644341
H 0.008055 -0.834886 -3.037730
H -0.083073 -2.201174 -0.713617

78-H$^+$
C -3.032399 1.288551 -0.206372
C -2.656246 -0.061091 0.002257
C -3.459523 -1.155101 -0.392501
C -4.680580 -0.864520 -1.028041
C -5.084403 0.457023 -1.246588
C -4.269214 1.518218 -0.834274

N -1.363631 -0.328722 0.631587
Si 0.011411 -0.706892 -0.426883
Cl -0.020201 0.359649 -2.166703
C -3.055621 -2.609498 -0.158396
C -2.780895 -3.323620 -1.503101
C -2.175422 2.479412 0.225452
C -1.863715 3.417589 -0.963970
C -1.237605 -0.341289 1.988180
C -2.494358 -0.306677 2.816184
C 0.016647 -0.392818 2.620048
C 1.263234 -0.283292 1.978733
C 2.523085 -0.195003 2.798358
N 1.377372 -0.273612 0.621911
C 2.662497 0.004621 -0.017921
C 2.976733 1.351372 -0.324222
C 4.226637 1.594940 -0.920294
C 5.105531 0.546936 -1.221781
C 4.751903 -0.774274 -0.928033
C 3.523993 -1.076914 -0.311547
C 2.033192 2.517233 -0.023770
C 1.877691 3.462732 -1.236760
C 3.166480 -2.530627 -0.006995
C 2.921020 -3.313070 -1.319455
C 4.256695 -3.227895 0.839648
C 2.509152 3.319311 1.211815
C -4.127899 -3.373298 0.653191
C -2.865542 3.285554 1.352802
H 3.139324 -1.089825 2.613082
H 5.436428 -1.587381 -1.172989
H 6.066656 0.761871 -1.691687
H 4.508438 2.620403 -1.160650
H 2.233119 -2.553435 0.577367
H 3.940776 -4.253598 1.085080
H 5.205557 -3.289854 0.285374
H 4.450238 -2.687235 1.779988
H 2.624411 -4.349572 -1.093726
H 2.130026 -2.844996 -1.926889
H 3.838654 -3.342562 -1.927342
H 1.035286 2.113838 0.206908
H 1.830314 4.167852 1.392739
H 2.532196 2.700925 2.122163
H 3.521251 3.719179 1.042930
H 1.119560 4.227654 -1.011361
H 2.821665 3.983705 -1.458406
H 1.565955 2.913279 -2.136588
H -4.591181 2.546086 -1.005834
H -6.037128 0.661527 -1.737761
H -5.320413 -1.688231 -1.347570
H -2.125429 -2.631105 0.431005
H -2.449304 -4.358392 -1.322735
H -3.695409 -3.358004 -2.115416
H -2.005143 -2.802192 -2.086513
H -3.789161 -4.402867 0.846788
H -4.328037 -2.883173 1.619565
H -5.077049 -3.426501 0.098376
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H -2.224126 4.127074 1.659093
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H -3.069143 2.669624 2.242018
H -1.212861 4.238846 -0.626047
H -1.359509 2.882437 -1.780107
H -2.788138 3.863370 -1.362240
H -2.256079 -0.321733 3.886722
H -3.091720 0.586629 2.585835
H -3.123579 -1.175696 2.564749
H 0.021728 -0.434969 3.706208
H 3.130741 0.669771 2.497088
H 2.288792 -0.129161 3.867840
H 0.043943 -2.134702 -0.784068

79-H$^+$
C 3.089464 1.282503 1.312987
C 2.257408 1.714417 0.249360
C 2.766116 2.271982 -0.948030
C 4.163415 2.374117 -1.072141
C 5.012829 1.946178 -0.046147
C 4.477746 1.414894 1.133443
N 0.815362 1.505047 0.357037
Si 0.232333 0.022744 -0.382917
O 1.131856 -1.250543 0.267652
S 1.671618 -2.618133 -0.521789
O 0.847424 -2.854925 -1.709314
C 1.871219 2.776843 -2.079888
C 2.128711 2.008733 -3.397578
C 2.555308 0.728328 2.635356
C 3.083587 -0.694671 2.934038
C -0.003936 2.399832 0.989092
C 0.604562 3.695889 1.452653
C -1.362856 2.152422 1.185284
C -2.065121 0.972387 0.837764
C -3.510983 0.879173 1.147174
Si -4.581809 2.191022 0.130735
C -4.685013 3.765720 1.187389
N -1.438567 -0.046114 0.178655
C -2.009914 -1.390093 0.069290
C -1.951824 -2.228098 1.214003
C -2.410518 -3.548204 1.065688
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C -2.928184 -3.169370 -1.272689
C -2.496764 -1.833257 -1.182191
C -1.451281 -1.756406 2.579791
C -0.343372 -2.674354 3.145054
C -2.599848 -0.928960 -2.407492
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C -4.074156 -0.799256 -2.858518
C -2.628954 -1.666449 3.580982
C 3.364948 -1.935190 -1.107273
F 3.936942 -2.864302 -1.871305
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F 3.147628 -0.816162 -1.822230
F 4.127857 -1.657945 -0.049728
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H -1.807484 -0.752091 -4.432542
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H -1.019533 -0.749695 2.478008
H -2.273033 -1.278632 4.548669
H -3.428832 -1.008010 3.210304
H -3.061265 -2.664881 3.751086
H 0.017562 -2.266380 4.102585
H -0.731028 -3.686615 3.337523
H 0.503706 -2.756695 2.452733
H 5.145161 1.093734 1.934198
H 6.094538 2.032908 -0.162431
H 4.583772 2.798393 -1.984952
H 0.817825 2.620577 -1.799110
H 1.465411 2.389794 -4.189861
H 3.169407 2.146442 -3.729756
H 1.950320 0.929961 -3.279986
H 1.386093 4.655160 -3.085498
H 1.877658 4.869098 -1.379841
H 3.101344 4.509600 -2.621584
H 1.457272 0.673031 2.583295
H 2.492442 1.282949 4.746706
H 4.029239 1.687980 3.941153
H 2.592958 2.696652 3.661766
H 2.687422 -1.036689 3.902948
H 2.781489 -1.413635 2.165121
H 4.182741 -0.694998 3.000450
H -0.150170 4.330813 1.932885
H 1.426672 3.509010 2.157302
H 1.042033 4.230372 0.594593
H -1.939769 2.930279 1.678865
H -3.901108 -0.130627 0.969410
H -3.682417 1.142211 2.202998
H -4.267750 3.401933 -2.030800
H -2.692953 2.917708 -1.365308
H -3.720689 1.721318 -2.202746
H -6.967639 2.080799 -0.625486
H -6.236025 0.458872 -0.664494
H -6.749350 1.169207 0.886930
H -5.383362 4.486459 0.728894
H -5.051405 3.555432 2.206386
H -3.709924 4.274341 1.272909
H 0.346923 -0.005775 -1.841686

80-H$^+$
C -0.746145 0.719180 -2.172995

C -1.096328 -0.465861 -1.502129
C -0.425747 -1.609391 -1.966683
C 0.511440 -1.590249 -3.014815
C 0.775363 -0.390687 -3.678480
C 0.155832 0.785537 -3.239172
B -2.033339 -0.369164 -0.139818
C -1.013908 0.578284 1.021533
C 0.388526 0.312130 0.862262
N 1.309887 1.369523 0.786299
C 1.001640 2.713635 1.304885
C 0.805722 2.829704 2.706382
C 0.587549 4.122480 3.212179
C 0.583539 5.243173 2.373973
C 0.787754 5.090782 0.999395
C 0.989544 3.821835 0.423419
C 0.835537 1.654412 3.685160
C 2.005995 1.807494 4.686393
C 1.189941 3.708158 -1.086883
C 2.611573 4.163801 -1.497962
F -0.567831 -2.813249 -1.354071
F 1.215102 -2.699208 -3.335815
F 1.661995 -0.340537 -4.693448
F 0.485424 1.958276 -3.824551
F -1.267504 1.897556 -1.748911
C -2.482320 -1.835255 0.472302
C -2.263703 -2.379809 1.745875
C -2.803073 -3.599623 2.184872
C -3.622004 -4.336629 1.322172
C -3.873550 -3.844605 0.032143
C -3.308899 -2.623644 -0.353301
F -1.448634 -1.752675 2.658669
F -3.575862 -2.202173 -1.613705
F -4.645535 -4.547095 -0.812190
F -4.147344 -5.504320 1.717919
F -2.534561 -4.062967 3.419656
C -3.405636 0.518717 -0.263309
C -4.042081 0.857865 -1.472608
C -5.255771 1.557722 -1.537203
C -5.896429 1.944141 -0.351380
C -5.316633 1.613537 0.881851
C -4.107521 0.907954 0.894980
F -3.510002 0.494705 -2.662244
F -5.814076 1.854853 -2.722451
F -7.054626 2.615416 -0.395395
F -5.926473 1.963941 2.027507
F -3.619455 0.590833 2.129249
C 0.860210 -1.030564 0.714374
C 2.124441 -1.475005 0.380756
N 3.187523 -0.576165 0.236046
C 4.574100 -0.987531 0.018491
C 5.358608 -1.293158 1.152777
C 6.710763 -1.608509 0.921076
C 7.236549 -1.618248 -0.375151
C 6.422372 -1.321205 -1.478537
C 5.065389 -0.999625 -1.308248
C 4.804357 -1.268476 2.576541

C 5.375076 -0.058584 3.355140
C 4.143371 -0.677347 -2.488985
C 3.897398 0.840782 -2.614721
C 2.397375 -2.924327 0.099520
Si 2.934461 1.094123 0.374649
C -0.513628 1.516055 4.430586
C 0.145228 4.538657 -1.870962
C 5.094802 -2.588352 3.327510
C 4.668292 -1.223371 -3.835943
H 0.426392 4.244873 4.283814
H 0.417218 6.236587 2.793326
H 0.775462 5.966367 0.350972
H 1.001653 0.714952 3.139491
H -0.497538 0.615660 5.063573
H -0.688262 2.387834 5.080012
H -1.358552 1.437193 3.731375
H 2.028587 0.943719 5.369246
H 2.976586 1.870649 4.166878
H 1.887419 2.718879 5.291965
H 1.059589 2.657844 -1.382620
H 0.203767 4.285372 -2.937247
H -0.873062 4.332399 -1.518886
H 0.343996 5.615920 -1.762451
H 2.746391 4.037357 -2.583486
H 2.756997 5.226633 -1.250238
H 3.409747 3.601276 -0.983196
H 6.847752 -1.351810 -2.480472
H 8.287565 -1.865496 -0.532019
H 7.352029 -1.848456 1.769719
H 3.709598 -1.156190 2.535704
H 4.954641 -0.028575 4.372025
H 6.470828 -0.131369 3.434150
H 5.140402 0.896391 2.853917
H 4.630466 -2.556921 4.324919
H 4.692928 -3.456404 2.782240
H 6.176681 -2.739067 3.462191
H 3.169900 -1.156517 -2.300737
H 3.901060 -1.101284 -4.607882
H 5.573620 -0.686635 -4.158871
H 4.909579 -2.292989 -3.747679
H 3.221740 1.078725 -3.446805
H 3.382213 1.255668 -1.694113
H 4.836262 1.406263 -2.710129
H 1.540880 -3.534608 0.408144
H 2.543446 -3.065538 -0.984841
H 3.309206 -3.269009 0.608414
H 0.093988 -1.793703 0.781689
H -1.387709 0.141184 1.949458
H -1.248461 1.645560 0.982229
H 4.012343 2.035754 0.669341

81-H$^+$
C 3.473731 1.398859 -0.599114
C 3.337950 0.034087 -0.259175
C 3.788984 -1.026229 -1.074937
C 4.414621 -0.674891 -2.285071

C 4.576159 0.665813 -2.653258
C 4.109675 1.689144 -1.818783
N 2.698781 -0.290690 1.001301
C 1.374608 -0.573887 1.131835
N 1.189213 -0.740662 2.480933
C 2.388253 -0.583768 3.175871
C 3.337306 -0.301178 2.235111
C -0.040955 -1.277096 3.056057
N -1.218377 -0.641416 2.470985
C -1.383005 -0.481232 1.118353
N -2.683178 -0.107919 0.973385
C -3.330263 -0.061587 2.201770
C -2.409835 -0.396568 3.153786
C -3.304924 0.170450 -0.307362
C -3.277511 1.500350 -0.787404
C -3.907928 1.739684 -2.020195
C -4.520121 0.700045 -2.733947
C -4.511987 -0.605408 -2.231866
C -3.900103 -0.904720 -1.000265
C -2.628827 2.630892 0.008228
C -1.911623 3.660319 -0.890346
C -3.903278 -2.339070 -0.476436
C -3.135317 -3.276335 -1.437612
Si 0.007886 -0.343217 -0.252084
C 3.648002 -2.496965 -0.690065
C 5.040150 -3.139263 -0.481664
C 2.955030 2.534020 0.280314
C 4.116324 3.432092 0.766079
C 2.835002 -3.276005 -1.749660
C 1.887290 3.364790 -0.468664
C -5.348704 -2.841227 -0.251913
C -3.684210 3.329341 0.900157
H 4.397651 -0.095931 2.321514
H 2.451378 -0.688856 4.253215
H 4.780134 -1.467207 -2.939698
H 5.066256 0.914906 -3.596132
H 4.233617 2.731445 -2.115492
H 2.471548 2.104589 1.171157
H 1.488500 4.147978 0.196162
H 2.322858 3.858538 -1.351650
H 1.057564 2.723651 -0.802782
H 3.727655 4.234690 1.412655
H 4.861275 2.852349 1.334463
H 4.629753 3.900116 -0.088314
H 3.102783 -2.567525 0.263367
H 2.721600 -4.325892 -1.436114
H 1.834296 -2.837302 -1.882951
H 3.348817 -3.266217 -2.723621
H 4.929301 -4.194448 -0.185535
H 5.626998 -3.104325 -1.412908
H 5.610318 -2.612692 0.300302
H -0.085124 -2.362529 2.866674
H -0.037398 -1.089110 4.136265
H -2.488644 -0.484520 4.231619
H -4.376889 0.206820 2.276588
H -4.983771 -1.410111 -2.797327

H -5.001391 0.910775 -3.690608
H -3.913641 2.749618 -2.429819
H -1.863983 2.190353 0.667290
H -3.214715 4.136550 1.484964
H -4.478602 3.769824 0.276885
H -4.154286 2.621098 1.600885
H -1.353283 4.369929 -0.260800
H -1.206131 3.164115 -1.573104
H -2.630332 4.242150 -1.488335
H -3.387101 -2.367840 0.495401
H -5.333378 -3.867578 0.147463
H -5.890606 -2.195519 0.457452
H -5.909425 -2.851731 -1.199487
H -3.125074 -4.301401 -1.033943
H -3.619670 -3.304073 -2.426246
H -2.095714 -2.939204 -1.572188
H -0.035588 -1.792391 -0.703273

82-H$^+$
C 3.151133 -1.246108 -0.048592
C 2.479418 -0.016579 0.140995
C 3.040306 1.249493 -0.124957
C 4.356766 1.260416 -0.623298
C 5.058213 0.067914 -0.831328
C 4.463252 -1.169679 -0.545713
N 1.109081 -0.061600 0.624463
C 0.021924 0.002981 -0.161163
N -1.073348 -0.041212 0.613562
C -0.675874 -0.137100 1.939915
C 0.695872 -0.147452 1.947075
C -2.439344 0.000007 0.118802
C -3.078866 -1.228971 -0.148430
C -4.393925 -1.157372 -0.642375
C -5.019762 0.077208 -0.855178
C -4.345713 1.273618 -0.577048
C -3.031733 1.266675 -0.075620
C -2.405296 -2.584627 0.054572
C -3.191746 -3.451383 1.065363
C -2.292503 2.577366 0.189492
C -3.126577 3.549510 1.054108
C 2.283443 2.560403 0.081386
C 1.983504 3.230254 -1.280628
C 2.464857 -2.588605 0.210119
C 1.705704 -3.048315 -1.060036
C 3.060979 3.523578 1.007810
C 3.437809 -3.690357 0.681044
C -1.892484 3.240756 -1.150530
C -2.243311 -3.322054 -1.295656
H 1.416769 -0.204706 2.753852
H -1.406285 -0.187615 2.738487
H 4.830512 2.217128 -0.845607
H 6.078607 0.099793 -1.216700
H 5.026546 -2.087667 -0.710037
H -4.841982 2.228963 -0.749752
H -6.039797 0.107963 -1.241625
H -4.925844 -2.083305 -0.864421

H 1.719477 -2.449661 1.010245
H 2.865210 -4.582996 0.974519
H 4.124888 -3.988792 -0.125816
H 4.036799 -3.357716 1.542417
H 1.193490 -4.004722 -0.870341
H 0.949657 -2.310258 -1.372704
H 2.409721 -3.190048 -1.894904
H 1.318715 2.347270 0.569188
H 2.475263 4.442554 1.165193
H 3.261213 3.061494 1.986894
H 4.025095 3.809229 0.560116
H 1.415786 4.161083 -1.127095
H 2.919867 3.479748 -1.803297
H 1.395710 2.567209 -1.935824
H -1.366302 2.359932 0.745789
H -2.533607 4.450453 1.274868
H -4.037767 3.868990 0.525748
H -3.425906 3.083145 2.005306
H -1.343855 4.176825 -0.961974
H -1.252404 2.577541 -1.754533
H -2.789252 3.478180 -1.743664
H -1.396770 -2.428570 0.468904
H -2.675777 -4.412424 1.215771
H -3.284459 -2.945598 2.039358
H -4.205836 -3.663959 0.693373
H -1.733079 -4.285150 -1.138744
H -3.225613 -3.524407 -1.749879
H -1.653687 -2.725986 -2.010212
H 0.028481 0.086303 -1.239869

83-H$^+$
C -0.408200 2.732892 -0.595260
C 0.464344 1.653400 -0.326489
C 1.687546 1.862219 0.344472
C 2.036873 3.160383 0.743523
C 1.175701 4.235954 0.474599
C -0.043885 4.023245 -0.192876
P -0.004172 -0.007374 -0.858572
C -1.682143 -0.405045 -0.340495
C -2.192814 0.146051 0.854730
C -3.469703 -0.231938 1.292147
C -4.228661 -1.146603 0.543322
C -3.717731 -1.690542 -0.648039
C -2.441789 -1.325714 -1.095588
C 1.188993 -1.244054 -0.313024
C 2.408322 -1.388483 -1.011989
C 3.355201 -2.312655 -0.552113
C 3.087293 -3.085043 0.591619
C 1.872109 -2.940026 1.281132
C 0.915041 -2.019048 0.833429
H 2.617334 -0.791955 -1.903093
H 4.296874 -2.434244 -1.088963
H 3.826790 -3.806460 0.942309
H 1.666130 -3.546990 2.163627
H -0.034616 -1.910019 1.360035
H -1.605867 0.867766 1.424885

H -3.872721 0.191997 2.212794
H -5.224037 -1.433311 0.885846
H -4.313861 -2.394271 -1.230289
H -2.046992 -1.750583 -2.021273
H 2.353476 1.023830 0.552339
H 2.980044 3.328865 1.264750
H 1.452814 5.243973 0.786839
H -0.711079 4.861436 -0.397881
H -1.360877 2.567625 -1.102613
H 0.000199 -0.057001 -2.269325

84-H$^+$
C -1.975318 -0.981115 1.097080
C -1.654018 -0.947502 -0.420755
C -2.794528 -0.278113 -1.232762
C -4.124927 -1.022810 -0.977753
C -4.458945 -1.070548 0.526809
C -3.313703 -1.717327 1.331885
P -0.034693 -0.129265 -0.734320
C -0.077715 1.653253 -0.247520
C 0.697458 2.546768 -1.254353
C 0.576627 4.030058 -0.841335
C 1.059113 4.254911 0.605631
C 0.289831 3.355055 1.593276
C 0.418914 1.864184 1.209260
C 1.359317 -1.044104 0.045834
C 2.725569 -0.493257 -0.447775
C 3.884345 -1.261947 0.225223
C 3.771736 -2.778154 -0.025771
C 2.412282 -3.316768 0.461591
C 1.233848 -2.571228 -0.204989
H 1.268013 -0.851660 1.128707
H 2.789854 -0.620037 -1.542868
H 2.809124 0.582750 -0.232393
H 4.840720 -0.873844 -0.157174
H 3.862626 -1.064060 1.311337
H 3.879308 -2.978698 -1.106371
H 4.590484 -3.306727 0.485264
H 2.320678 -4.392826 0.249265
H 2.337856 -3.191986 1.556205
H 1.246326 -2.764934 -1.292540
H 0.278686 -2.949539 0.191287
H -1.145588 1.931387 -0.291421
H 1.760636 2.253695 -1.263443
H 0.304898 2.400234 -2.273678
H 1.156106 4.647496 -1.544449
H -0.479497 4.340107 -0.929861
H 2.138047 4.027401 0.670744
H 0.933786 5.312110 0.884115
H 0.664191 3.494945 2.618928
H -0.778125 3.635209 1.594784
H 1.477337 1.563128 1.280534
H -0.153013 1.236358 1.910775
H -1.531634 -1.984167 -0.780269
H -2.905491 0.772628 -0.914471
H -2.555015 -0.277956 -2.308923

H -4.929322 -0.523189 -1.538616
H -4.041693 -2.050707 -1.371580
H -4.628028 -0.043117 0.895557
H -5.392977 -1.629741 0.687408
H -3.544329 -1.711612 2.408057
H -3.198272 -2.772522 1.028323
H -2.058621 0.053845 1.470385
H -1.163749 -1.473752 1.656875
H 0.187761 -0.179377 -2.127150

2.3. Structures with connected =P-H units (initial states)

1-PH
C -3.899293 -1.025700 0.825307
C -3.154250 -0.095960 0.055845
C -3.714180 1.156273 -0.314667
C -5.027585 1.450365 0.091210
C -5.779916 0.536995 0.838412
C -5.213360 -0.689658 1.199295
N -1.796968 -0.408126 -0.351984
Si -1.614839 -1.340305 -1.875117
C -0.272021 -0.505088 -2.921603
C -2.923893 2.205355 -1.095292
C -3.680131 2.700305 -2.349003
C -3.326731 -2.372563 1.260602
C -3.288493 -2.509538 2.799943
Si -0.554585 0.139738 0.742191
B 1.356190 0.153174 0.118514
N 2.322901 -0.917050 -0.060778
C 2.165335 -2.339008 0.054818
C 1.833699 -2.893134 1.321951
C 1.646914 -4.284924 1.401239
C 1.829799 -5.109807 0.284275
C 2.212225 -4.549843 -0.937169
C 2.377216 -3.159568 -1.082440
C 1.813220 -2.036612 2.589245
C 0.920791 -2.591103 3.714760
C 2.801131 -2.602316 -2.442005
C 4.291361 -2.921884 -2.713368
C 3.576763 -0.347010 -0.326585
C 3.461219 1.011407 -0.334007
N 2.134495 1.362210 -0.059219
C 1.742256 2.741960 0.054298
C 1.332809 3.434537 -1.109786
C 0.973897 4.789024 -0.981142
C 1.017402 5.428660 0.262093
C 1.431305 4.724731 1.399473
C 1.806281 3.371252 1.323257
C 1.343119 2.761192 -2.479425
C 2.666283 3.073772 -3.218152
C 2.317551 2.628057 2.557886
C 1.690978 3.119846 3.878853
C 3.264695 -1.824400 3.084946
C 1.938790 -3.145255 -3.603671
C 3.860787 2.729219 2.648235
C 0.136008 3.151496 -3.357022

C -2.560251 3.404997 -0.187366
C -4.129116 -3.538637 0.637921
C -1.173405 -3.149738 -1.513552
C -3.276919 -1.283723 -2.785396
H -3.205973 -1.855404 -3.727232
H -4.082941 -1.724499 -2.177720
H -3.575515 -0.253182 -3.031004
H -0.164347 -0.997326 -3.902472
H -0.533034 0.549459 -3.097349
H 0.708656 -0.533368 -2.422593
H -0.996240 -3.702531 -2.452264
H -0.265793 -3.246112 -0.899957
H -1.996257 -3.654478 -0.985668
H -5.461300 2.414765 -0.181220
H -6.799752 0.783009 1.142677
H -5.792050 -1.403331 1.789873
H -1.984188 1.744928 -1.431311
H -1.934287 4.125429 -0.738326
H -3.476900 3.919731 0.146337
H -2.003862 3.073269 0.701510
H -3.055431 3.417896 -2.905637
H -3.940547 1.869336 -3.023297
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H -2.291345 -2.438644 0.902087
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10-PH

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H 0.120937 4.686515 -2.890851
P 1.248507 -0.501514 -2.676345
H -0.173234 -0.637694 -2.834021

16-PH
C -3.941471 -1.412765 0.121311
C -3.394655 -0.163613 0.523108
C -3.522175 0.291924 1.863450
C -4.253258 -0.497816 2.768803
C -4.834228 -1.706776 2.379298
C -4.663075 -2.159838 1.068759
N -2.757701 0.691567 -0.460294
C -1.407902 0.791534 -0.678501
C -1.200176 2.018043 -1.611163
C -2.590693 2.211293 -2.260493
C -3.615423 1.658240 -1.250244
Si -0.038057 0.076276 0.397967
P -0.401648 -1.906084 1.346234
C -4.770283 0.941719 -1.969732

C -4.249993 2.737318 -0.349007
C -0.837151 3.246335 -0.731636
C -0.089330 1.890498 -2.677466
C -2.842385 1.550418 2.405951
C -3.839899 2.546531 3.043173
C -3.719574 -2.037826 -1.256570
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C 1.312387 -0.613909 -0.774616
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C 3.445867 -0.785847 -1.916332
C 2.318021 -1.249863 -2.863108
C 1.120993 -1.611953 -1.954337
C 3.423355 0.189554 0.421732
C 3.801213 1.561212 0.436326
C 4.836299 1.966892 1.300228
C 5.467853 1.067380 2.160899
C 5.004533 -0.248216 2.222381
C 3.977120 -0.711026 1.378821
C 3.051080 2.659484 -0.314115
C 3.952537 3.565236 -1.185086
C 3.443522 -2.119400 1.635957
C 4.510130 -3.234172 1.529995
C 1.250395 -3.089421 -1.471087
C -0.220218 -1.518167 -2.700047
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C 4.481943 -1.882760 -1.621701
C 2.843966 -2.164013 3.066314
C 2.330737 3.542709 0.739039
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H -4.348563 -0.158732 3.801921
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H -5.723772 -1.548575 -2.066784
H -2.631997 -3.711610 -2.143906
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H -1.227170 2.080650 3.776224
H -2.258471 0.742213 4.356729
H -1.059466 0.444710 3.067376
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H -4.321202 2.096119 3.926225
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H 3.647536 -2.111520 3.820247
H 2.152888 -1.327751 3.232792
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H 4.655867 0.117371 -3.455415
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H 5.190569 -1.544546 -0.852909
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17-PH
C -4.026661 -1.345510 0.502071
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C -1.179195 1.864184 -1.476412
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C -3.604710 1.612145 -1.080313
C -0.718994 3.120130 -0.668541
C -0.465429 4.363116 -1.542826
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C 4.742431 2.106225 1.596232
C 3.774540 1.629099 0.690589
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C -1.772759 1.429323 3.661773
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H 5.042684 -2.816242 3.081534
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H -4.958370 -2.917342 -2.496525
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H -2.275854 2.164720 1.712741
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H -2.264644 1.053243 4.573423
H -1.059179 0.672486 3.313012
H -3.243770 3.716618 3.391745
H -4.577123 3.083468 2.387752
H -4.304389 2.434277 4.020795
H 0.818209 1.260755 -2.098220
H -0.470035 0.783640 -3.223995
H 0.918588 2.578083 -4.207414
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H 1.541277 3.860555 -2.177479
H 0.692733 4.935458 -3.306293
H -0.110765 5.186246 -0.899563
H -1.407761 4.709120 -2.001789
H 0.204381 2.833625 -0.158933
H -1.449023 3.350810 0.118926
H -0.939584 -2.040097 -1.460224
H -0.323125 -0.964008 -2.710674
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H -5.353731 1.612628 -2.341734
H -4.418642 0.095755 -2.428810
H -5.440973 0.437676 -1.000592
P -0.532742 -1.888427 1.771050
H -0.307042 -1.348987 3.083886

18-PH

C	-2.523370	-3.270914	-0.774166
C	-2.007624	-1.901320	-1.116581
C	-3.161238	-0.974753	-0.785238
C	-4.159390	-1.727515	-0.215114
C	-3.763028	-3.137117	-0.200627
Si	-0.841018	-1.432406	0.353205

P	-0.959449	-2.533474	2.163680
N	0.092634	-0.118636	-0.085144
C	0.988136	0.787624	0.083105
N	0.762744	2.142917	0.331145
C	1.975889	2.834373	0.381559
C	2.970419	1.933185	0.166977
N	2.378352	0.677971	-0.011188
C	-0.541404	2.743460	0.376692
C	-0.981410	3.480232	-0.748971
C	-2.260480	4.061273	-0.682944
C	-3.068511	3.894267	0.447601
C	-2.615286	3.139872	1.536710
C	-1.339743	2.547914	1.528159
C	-0.146027	3.550620	-2.028332
C	-0.425432	2.295661	-2.890850
C	-0.816136	1.746055	2.719354
C	0.170447	2.600507	3.551153
C	3.096198	-0.552056	-0.207479
C	3.837886	-1.081718	0.877460
C	4.530458	-2.286548	0.659392
C	4.481609	-2.933219	-0.580569
C	3.750740	-2.379674	-1.638011
C	3.047620	-1.171825	-1.480073
C	3.854360	-0.389585	2.244532
C	5.043380	-0.798987	3.136885
C	2.299890	-0.522320	-2.646397
C	2.004294	-1.487390	-3.811445
C	2.522040	-0.637050	2.987659
C	3.079466	0.705122	-3.179351
C	-1.928148	1.175312	3.620075
C	-0.373547	4.834493	-2.852118
C	-1.711739	-4.520596	-0.968255
C	-4.611550	-4.216531	0.415532
C	-5.460019	-1.241709	0.364583
C	-3.170703	0.488119	-1.133832
C	-1.375646	-1.720421	-2.505822
H	2.000991	3.903076	0.555638
H	4.045800	2.051473	0.120630
H	-3.262739	3.002494	2.402211
H	-4.062591	4.345979	0.475960
H	-2.633132	4.635726	-1.531214
H	0.918793	3.526010	-1.754081
H	0.345143	4.868175	-3.686190
H	-1.385724	4.860234	-3.287367
H	-0.239693	5.738226	-2.236365
H	0.234712	2.283276	-3.773859
H	-0.262251	1.377124	-2.310849
H	-1.472463	2.297447	-3.234446
H	-0.263009	0.884085	2.323213
H	-1.478392	0.502490	4.365373
H	-2.459651	1.976271	4.161373
H	-2.654666	0.593840	3.033221
H	0.572205	2.002694	4.385506
H	1.015228	2.949917	2.938301
H	-0.344571	3.480816	3.970556
H	3.730089	-2.891601	-2.599584

H	5.019483	-3.872757	-0.724504
H	5.109352	-2.728214	1.470012
H	3.936533	0.695830	2.078873
H	5.054466	-0.169632	4.040374
H	4.955169	-1.847860	3.463755
H	6.005564	-0.679526	2.613421
H	2.515465	-0.095939	3.948383
H	1.664646	-0.301061	2.391028
H	2.386589	-1.711179	3.186031
H	1.331681	-0.172539	-2.264742
H	1.331919	-0.994990	-4.530504
H	2.927499	-1.764852	-4.346739
H	1.518215	-2.409345	-3.459269
H	2.517811	1.177732	-4.002093
H	3.238989	1.459520	-2.395579
H	4.062933	0.392138	-3.567756
H	-0.071554	-1.618614	2.827857
H	-2.325778	-5.421954	-0.821409
H	-1.280876	-4.565127	-1.984799
H	-0.870273	-4.570447	-0.253134
H	-4.196078	-5.218017	0.230576
H	-4.679187	-4.079122	1.509613
H	-5.643642	-4.192525	0.023222
H	-6.324357	-1.750470	-0.098352
H	-5.508158	-1.457258	1.447600
H	-5.589202	-0.157636	0.229254
H	-2.139202	-1.881125	-3.285859
H	-0.963307	-0.708230	-2.620953
H	-0.559696	-2.440569	-2.664767
H	-4.080057	0.983578	-0.763817
H	-2.303790	1.019885	-0.715037
H	-3.129775	0.631541	-2.230017

19-PH

C	0.726510	3.147808	-1.440750
C	1.004224	2.269000	-0.245271
C	0.215530	2.917280	0.877893
C	-0.450596	4.002514	0.363502
C	-0.146834	4.134984	-1.064621
Si	-0.042419	0.654988	-0.532355
P	-1.229698	0.663617	-2.276633
C	-0.009289	-0.730607	0.799586
C	-1.237327	-1.248465	1.315017
C	-1.228637	-2.172097	2.379045
C	-0.029668	-2.677316	2.888735
C	1.173898	-2.287342	2.295429
C	1.208636	-1.321573	1.268631
C	-2.568720	-1.045945	0.649032
C	-3.404023	0.062895	0.930883
C	-4.654320	0.145674	0.301371
C	-5.099793	-0.840082	-0.595576
C	-4.263138	-1.933337	-0.850970
C	-2.998754	-2.058345	-0.248737
C	-2.945701	1.127936	1.924409
C	-3.577345	2.511540	1.688416
C	-2.134021	-3.279297	-0.582403

C	-1.994084	-3.518374	-2.102863
C	-6.453731	-0.711104	-1.282967
C	-7.609120	-0.725607	-0.255841
C	2.531562	-1.055820	0.620063
C	3.637516	-0.567481	1.371061
C	4.847432	-0.302871	0.705400
C	4.997955	-0.497850	-0.671619
C	3.922412	-1.056432	-1.382152
C	2.702484	-1.373496	-0.765304
C	3.581597	-0.313707	2.883481
C	4.083815	1.086820	3.310058
C	6.285630	-0.109983	-1.386865
C	6.017575	1.027201	-2.401234
C	1.677583	-2.225913	-1.530536
C	1.696165	-2.035300	-3.059102
C	4.414316	-1.391377	3.621267
C	6.940617	-1.321525	-2.088611
C	1.903407	-3.713062	-1.162751
C	-2.698027	-4.540359	0.111713
C	-6.515469	0.563668	-2.155582
C	-3.208138	0.666453	3.377678
C	-1.305388	4.995362	1.103613
C	-0.743122	5.215653	-1.925811
C	1.402909	2.943297	-2.765728
C	2.505943	2.145209	0.059366
C	0.356423	2.502317	2.318883
H	-2.185626	-2.532522	2.759962
H	-0.035314	-3.410776	3.697923
H	2.111412	-2.744659	2.611228
H	5.692598	0.093319	1.273151
H	4.053365	-1.268991	-2.442967
H	-4.601140	-2.703271	-1.548937
H	-5.298827	1.002607	0.498471
H	-1.121169	-3.112705	-0.191098
H	-1.323312	-4.375095	-2.281114
H	-2.965787	-3.750638	-2.567329
H	-1.573353	-2.634632	-2.605511
H	-2.072945	-5.419327	-0.119256
H	-2.724773	-4.407807	1.204549
H	-3.724791	-4.743576	-0.234930
H	-6.578032	-1.584546	-1.946628
H	-7.485614	0.628115	-2.676085
H	-6.401037	1.464721	-1.531059
H	-5.708765	0.566195	-2.905169
H	-8.583087	-0.662309	-0.769261
H	-7.588384	-1.646226	0.348837
H	-7.527888	0.134302	0.429314
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H	-3.115601	3.246967	2.362954
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H	-4.658970	2.499480	1.901992
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H	0.855164	-2.591658	-3.500723

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H	1.159492	-4.345331	-1.675388
H	2.911379	-4.037838	-1.470285
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H	2.539213	-0.398651	3.219156
H	4.023838	1.175882	4.407124
H	5.133953	1.245996	3.018894
H	3.480473	1.892972	2.869361
H	4.330176	-1.261319	4.713008
H	4.085929	-2.409912	3.362803
H	5.477700	-1.304286	3.344068
H	6.992199	0.267906	-0.627611
H	6.952330	1.326286	-2.904005
H	5.303737	0.692498	-3.171517
H	5.588569	1.909340	-1.899714
H	7.887309	-1.021737	-2.567465
H	7.149512	-2.129496	-1.369712
H	6.276129	-1.723000	-2.870876
H	-1.888190	-0.555842	-1.927581
H	-0.322831	5.206411	-2.941867
H	-1.836528	5.084718	-2.014024
H	-0.574782	6.216840	-1.491229
H	1.158032	3.752380	-3.469659
H	2.501070	2.916691	-2.641713
H	1.109341	1.988119	-3.236160
H	2.932626	3.159698	0.142796
H	2.662051	1.623652	1.004030
H	3.041801	1.591575	-0.723098
H	-2.326037	5.039616	0.687415
H	-1.384747	4.748508	2.171687
H	-0.881403	6.011973	1.019283
H	-0.439431	2.936939	2.942383
H	0.318999	1.407429	2.439832
H	1.326693	2.835066	2.733451

20-PH

C	2.412933	-0.880598	0.790262
C	1.594275	0.397846	0.839926
C	2.324988	1.333467	-0.093919
C	3.383640	0.663162	-0.643646
C	3.437815	-0.702141	-0.098740
Si	-0.027014	-0.121138	-0.123413
P	-0.092291	-0.498769	-2.196462
C	-1.646618	-0.384818	0.925871
C	-2.283303	0.984727	0.763832
C	-3.299707	0.878913	-0.152377
C	-3.421757	-0.512964	-0.593251
C	-2.486386	-1.281223	0.051748
C	-1.855295	2.211117	1.527829
C	-4.164327	1.982527	-0.696974
C	-4.422050	-0.956845	-1.625996
C	-2.245297	-2.759084	-0.072195
C	-1.492472	-0.875381	2.379347
C	1.873593	2.744655	-0.344315
C	4.366191	1.169651	-1.665460

C	4.472593	-1.706514	-0.528449
C	2.080436	-2.102350	1.604255
C	1.429818	0.966450	2.267067
H	1.253189	-0.006215	-2.336874
H	-5.441832	-0.621312	-1.368353
H	-4.180506	-0.523246	-2.612740
H	-4.436549	-2.050805	-1.736427
H	-5.235870	1.729275	-0.616998
H	-3.995692	2.935286	-0.173762
H	-3.955538	2.145926	-1.769879
H	-2.638335	2.983667	1.495857
H	-1.660098	1.974105	2.587958
H	-0.932998	2.668796	1.126465
H	-3.088757	-3.259057	-0.571319
H	-1.335629	-2.971710	-0.663284
H	-2.111268	-3.226799	0.919259
H	-0.914308	-1.810107	2.437536
H	-0.997810	-0.123840	3.008212
H	-2.495280	-1.062801	2.798177
H	4.404113	-2.639915	0.049229
H	4.350552	-1.962349	-1.596630
H	5.494438	-1.304428	-0.413336
H	5.406663	1.041943	-1.318556
H	4.276125	0.606481	-2.611709
H	4.208796	2.234224	-1.892215
H	2.630682	3.315878	-0.902067
H	0.936719	2.774244	-0.932022
H	1.678464	3.277559	0.603686
H	2.419807	1.292736	2.626954
H	0.748275	1.827638	2.294956
H	1.052179	0.204122	2.961478
H	2.900450	-2.835218	1.574211
H	1.896318	-1.845372	2.662574
H	1.171846	-2.614816	1.235428

21-PH

C -0.132268 -2.456480 1.517507
Si 0.020680 -1.366256 -0.020608
C 0.187451 -2.418120 -1.584929
Si -0.007081 1.177913 -0.002619
N 1.216831 -0.055748 0.127637
C 2.691555 -0.026424 0.034450
C 3.248200 1.015066 1.028759
N -1.197920 -0.080328 -0.142151
C -2.669793 -0.087516 -0.005796
C -3.265005 1.088566 -0.808093
C -3.217160 -1.417725 -0.566902
C -3.054867 0.048413 1.485910
C 3.245790 -1.419498 0.403209
C 3.114178 0.340279 -1.406503
H -4.150884 0.051549 1.607750
H -2.639800 -0.790758 2.066366
H -2.654232 0.990006 1.893790
H -4.315763 -1.435237 -0.494831
H -2.929057 -1.536903 -1.622864
H -2.827429 -2.275755 0.006987

H -4.364307 1.079132 -0.733680
H -2.903254 2.052339 -0.415975
H -2.978059 1.012241 -1.868170
H 4.212715 0.375159 -1.496473
H 2.725695 -0.405578 -2.117977
H 2.708263 1.327692 -1.678893
H 4.348910 1.037035 0.980882
H 2.871822 2.021470 0.788243
H 2.940039 0.763983 2.055543
H 4.345969 -1.410565 0.362943
H 2.933348 -1.700192 1.421310
H 2.886624 -2.184781 -0.304511
H 0.723566 -3.147211 1.604656
H -0.164287 -1.834116 2.425986
H -1.049624 -3.068906 1.489112
H 1.090988 -3.050761 -1.561177
H -0.681512 -3.087443 -1.704285
H 0.243346 -1.771823 -2.475592
P -0.187413 3.278047 -0.038732
H 1.226866 3.408681 0.192955

22-PH
C 3.450003 0.004159 1.554714
C 2.069082 0.045961 1.311150
C 1.584438 -0.060534 -0.005861
C 2.487211 -0.207425 -1.076377
C 3.865554 -0.239427 -0.829196
C 4.349577 -0.134854 0.486042
C 0.121343 -0.008001 -0.262350
N -0.692490 -1.055872 -0.492412
C -0.497828 -2.494569 -0.181691
C 0.779404 -3.062162 -0.837266
N -0.638052 1.099174 -0.304590
Si -2.210018 0.082866 -0.531079
C -0.289366 2.536358 -0.217139
C -0.064236 2.911995 1.265318
C 0.957526 2.886263 -1.057873
C -1.507051 3.312545 -0.763243
C -0.445019 -2.676603 1.352677
C -1.729079 -3.230060 -0.751408
H -2.557757 0.188849 -1.981601
H 2.103094 -0.292095 -2.093809
H 4.562337 -0.347881 -1.662567
H 5.424181 -0.162952 0.676313
H 3.820814 0.081732 2.578478
H 1.364298 0.155602 2.136229
H -1.314425 4.393784 -0.688597
H -1.685550 3.057925 -1.819954
H -2.409753 3.068760 -0.182186
H 1.079205 3.981022 -1.069750
H 1.871592 2.443921 -0.640898
H 0.833662 2.537756 -2.095356
H 0.103438 3.997765 1.352474
H -0.948482 2.639469 1.860901
H 0.817862 2.391054 1.665584
H -1.639438 -4.307139 -0.542143

H -2.652392 -2.853265 -0.285277
H -1.792917 -3.086378 -1.841803
H -0.374373 -3.747906 1.601995
H 0.436622 -2.164773 1.768516
H -1.355917 -2.262235 1.810850
H 0.785626 -4.155848 -0.704772
H 0.791100 -2.841222 -1.916131
H 1.691566 -2.656869 -0.380518
P -3.652264 0.062242 1.032895
H -4.705728 0.042180 0.049725

23-PH
C 3.680486 0.045427 1.409465
C 2.286222 0.064760 1.256647
C 1.718089 -0.047163 -0.026297
C 2.551422 -0.176724 -1.153400
C 3.943344 -0.188063 -0.997106
C 4.510511 -0.078210 0.283977
C 0.239958 -0.011599 -0.181393
N -0.578506 -1.070085 -0.337608
C -0.337870 -2.509135 -0.074611
C 0.883660 -3.046097 -0.850885
N -0.530418 1.086866 -0.167249
Si -2.110371 0.046036 -0.232065
C -2.775569 0.168027 -2.007765
C -0.200277 2.525916 -0.082295
C 0.051012 2.896910 1.397168
C 1.020480 2.902765 -0.948910
C -1.443933 3.283304 -0.597206
C -0.150587 -2.724926 1.445053
C -1.605127 -3.249570 -0.553134
H 2.103711 -0.264962 -2.144244
H 4.585834 -0.284041 -1.874518
H 5.595565 -0.089424 0.403704
H 4.116406 0.128062 2.406889
H 1.634687 0.162031 2.126048
H -1.273132 4.367688 -0.515528
H -1.637840 3.034801 -1.652266
H -2.329025 3.016600 0.001538
H 1.119908 3.999762 -0.959171
H 1.952307 2.477139 -0.554615
H 0.880793 2.555240 -1.984793
H 0.208469 3.983925 1.489081
H -0.817811 2.608499 2.007710
H 0.946569 2.381893 1.775380
H -1.488790 -4.328809 -0.369399
H -2.490561 -2.888525 -0.007304
H -1.758704 -3.090016 -1.632315
H -0.039105 -3.799887 1.661789
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H -1.026218 -2.338837 1.988498
H 0.910927 -4.142723 -0.749630
H 0.800920 -2.796947 -1.920577
H 1.828052 -2.642562 -0.463718
H -3.346635 -0.737317 -2.270846
H -3.447683 1.033841 -2.120236

H -1.947094 0.273530 -2.727106
P -3.489077 -0.014729 1.386563
H -2.421704 -0.089970 2.356957

24-PH
C -4.120833 -0.295657 1.086607
C -2.720131 -0.231394 1.114499
C -2.002301 -0.013656 -0.076766
C -2.692931 0.133238 -1.294627
C -4.091535 0.054723 -1.320160
C -4.807784 -0.158069 -0.130223
C -0.517917 0.024963 -0.043118
N 0.269385 1.115528 -0.149960
C -0.065424 2.543139 0.092864
C -1.125246 3.053573 -0.906083
N 0.288342 -1.030157 0.138358
Si 1.810488 0.084138 0.284067
N 2.738219 0.055678 -1.179205
C 4.118766 -0.425890 -1.216653
C 0.042888 -2.488371 0.098829
C -0.455617 -2.959767 1.483671
C -0.965574 -2.878313 -1.002516
C 1.410114 -3.141196 -0.206401
C 2.133600 0.131858 -2.504005
C -0.553356 2.722084 1.547902
C 1.247607 3.327479 -0.115771
H -2.129701 0.302341 -2.213343
H -4.622523 0.161923 -2.267961
H -5.897787 -0.215119 -0.151887
H -4.673443 -0.455721 2.014318
H -2.177587 -0.340277 2.054392
H 1.299114 -4.236404 -0.217386
H 1.784994 -2.810347 -1.187403
H 2.147077 -2.863200 0.563404
H -0.997452 -3.976500 -1.080997
H -1.978679 -2.519471 -0.777724
H -0.649375 -2.468827 -1.975189
H -0.540885 -4.058529 1.495753
H 0.255468 -2.648799 2.263811
H -1.444262 -2.530888 1.703966
H 1.056120 4.402754 0.022296
H 2.005988 3.004258 0.613761
H 1.637220 3.162158 -1.132143
H -0.719124 3.790910 1.759437
H -1.501520 2.185369 1.706848
H 0.207300 2.332497 2.241866
H -1.228726 4.143935 -0.787708
H -0.811013 2.844218 -1.941191
H -2.107360 2.595301 -0.731616
H 4.754002 0.273002 -1.793977
H 4.522418 -0.511088 -0.197746
H 4.182386 -1.421944 -1.702996
H 2.744753 0.772297 -3.169320
H 2.061350 -0.869523 -2.980107
H 1.125061 0.565739 -2.440182
P 2.842282 0.202495 2.146030

H 1.637548 -0.205221 2.828999

25-PH
C -5.146930 -0.241035 -0.754098
C -4.714205 -0.119244 0.576536
C -3.344838 -0.044149 0.867053
C -2.402505 -0.076909 -0.178119
C -2.836739 -0.192900 -1.512010
C -4.206301 -0.280706 -1.796642
C -0.950350 0.003419 0.126700
N -0.190441 -0.998314 0.593563
C -0.372933 -2.467382 0.471186
C 0.850876 -3.113179 1.154776
N -0.164346 1.092524 -0.003214
Si 1.325059 0.121600 0.664949
O 2.158026 -0.520485 -0.632622
C 3.494003 -0.236169 -1.138142
C 4.541256 -0.789167 -0.155627
C -0.558161 2.528354 -0.010170
C 0.741942 3.337374 -0.194861
C -1.517709 2.849383 -1.177123
C -1.216066 2.895839 1.338957
C -1.661448 -2.940440 1.176535
C -0.395296 -2.854721 -1.024831
C 3.573004 -0.976584 -2.483808
C 3.674844 1.277545 -1.343580
H -2.099766 -0.206515 -2.316011
H -4.538742 -0.375359 -2.832149
H -6.213533 -0.304893 -0.977944
H -5.441990 -0.088557 1.389614
H -2.999069 0.032855 1.898684
H 0.754497 -4.208982 1.109818
H 1.775474 -2.816105 0.638803
H 0.919546 -2.798482 2.206764
H -0.428028 -3.951691 -1.125624
H -1.283854 -2.434757 -1.520538
H 0.509845 -2.472130 -1.518248
H -1.678231 -4.041946 1.182610
H -1.680926 -2.584956 2.218380
H -2.563329 -2.585560 0.660888
H 0.504424 4.412255 -0.180034
H 1.456912 3.113173 0.610961
H 1.211519 3.092921 -1.159939
H -1.458271 3.970677 1.355623
H -2.148479 2.328255 1.480096
H -0.528592 2.674875 2.169178
H -1.635840 3.942750 -1.243474
H -1.100310 2.485054 -2.128756
H -2.510730 2.405909 -1.029882
H 4.565008 -0.830709 -2.939968
H 3.407970 -2.055049 -2.333327
H 2.804866 -0.594114 -3.174171
H 4.667073 1.483943 -1.775934
H 2.904309 1.659233 -2.031775
H 3.591343 1.805744 -0.381712
H 5.553719 -0.648396 -0.568045

H 4.481852 -0.269485 0.812079
H 4.374403 -1.865515 0.007150
P 2.337005 0.723092 2.434943
H 1.125669 1.325213 2.935576

26-PH
C -4.996410 -0.185775 -0.717558
C -4.546952 -0.075524 0.608562
C -3.173375 -0.024731 0.884254
C -2.244019 -0.071250 -0.171761
C -2.694466 -0.176075 -1.501084
C -4.068297 -0.239264 -1.770643
C -0.787874 -0.007100 0.115072
N -0.027161 -1.019603 0.558780
C -0.220406 -2.485776 0.415441
C 0.994099 -3.150263 1.097254
N 0.003061 1.077927 -0.013221
Si 1.495717 0.089360 0.616809
O 2.324368 -0.534046 -0.697928
C 3.699718 -0.203527 -1.017244
C 3.732654 1.076022 -1.860596
C -0.375888 2.516999 0.012755
C 0.917912 3.311463 -0.259053
C -1.414460 2.860053 -1.077419
C -0.930322 2.878026 1.409507
C -1.517282 -2.958072 1.105511
C -0.236496 -2.850685 -1.086296
C 4.292065 -1.408636 -1.753544
H -1.966916 -0.199841 -2.313371
H -4.413851 -0.324809 -2.802634
H -6.066394 -0.229965 -0.929660
H -5.265192 -0.034417 1.429622
H -2.815183 0.043902 1.912276
H 0.890063 -4.244535 1.035652
H 1.924665 -2.853300 0.591835
H 1.058207 -2.851711 2.154198
H -0.280417 -3.945589 -1.203543
H -1.117556 -2.413833 -1.581001
H 0.676008 -2.470929 -1.568294
H -1.542998 -4.059323 1.094973
H -1.541143 -2.618053 2.152417
H -2.412790 -2.588153 0.589355
H 0.700154 4.389321 -0.206247
H 1.689024 3.061338 0.485874
H 1.304274 3.077912 -1.263247
H -1.169757 3.952878 1.451061
H -1.850344 2.309525 1.616350
H -0.183300 2.651116 2.184768
H -1.511245 3.955981 -1.134025
H -1.081811 2.488203 -2.058879
H -2.403550 2.440053 -0.853957
H 4.260146 -0.034597 -0.081451
H 5.347486 -1.217603 -2.006138
H 4.236797 -2.309611 -1.123395
H 3.733938 -1.594394 -2.685855
H 4.768427 1.323080 -2.145713

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H 3.317755 1.918281 -1.287060
P 2.613143 0.664278 2.329268
H 1.435856 1.256399 2.913553

27-PH
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C -5.321519 0.003842 -1.326909
C -5.119661 0.238676 0.043101
C -3.820839 0.256615 0.570095
C -1.332778 0.026066 0.275364
N -0.599554 1.107317 0.601097
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C 0.419958 3.302238 0.779911
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C 3.774933 -2.023872 0.040217
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C 0.200389 -3.218878 1.312807
C -2.246034 -2.693293 1.382389
C -1.102735 -3.072074 -0.848268
P 1.573450 0.097203 3.015570
C -1.025572 2.765499 -1.214604
C -2.057088 3.070718 1.086581
C 3.553236 1.131211 -0.949886
C 3.366417 2.369525 -1.854754
C 4.042372 1.541738 0.450819
C 3.429412 -1.952574 -2.476545
H -2.057794 -0.377892 -2.291966
H -4.371503 -0.396535 -3.235582
H -6.333554 -0.006070 -1.736305
H -5.972919 0.408952 0.702467
H -3.656154 0.434658 1.633253
H -0.043086 -4.290758 1.377518
H 1.153995 -3.111117 0.777407
H 0.333476 -2.806707 2.322867
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H -2.159842 -2.209554 2.367639
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H 0.591523 3.140790 1.853827
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H -1.952239 2.835873 2.156969
H -1.088617 3.846217 -1.421398
H -0.172662 2.344315 -1.768124
H -1.950171 2.290696 -1.571831
H 4.301255 2.956512 -1.886978

H 3.098066 2.082128 -2.883737
H 2.572030 3.030839 -1.472472
H 4.950490 2.164412 0.357405
H 3.280114 2.121458 0.992216
H 4.280384 0.665262 1.068272
H 4.335530 0.502292 -1.408703
H 1.923767 -2.403662 -1.013002
H 4.158124 -3.055461 -0.058562
H 4.639068 -1.341550 -0.003513
H 3.305621 -1.917622 1.030286
H 3.815763 -2.984896 -2.537762
H 2.707008 -1.799392 -3.293871
H 4.281375 -1.271996 -2.640152
H 2.935281 -0.161636 2.643564

28-PH
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C -3.143426 -0.272400 0.013283
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C -4.835082 -1.804490 -0.829358
C -5.841745 -1.023649 -0.239044
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N -0.786850 -0.370202 0.948780
C -0.974028 -1.200486 2.170212
C -1.367766 -2.642503 1.784291
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P 2.070287 0.358085 -0.902376
Si 3.982459 0.522514 0.325195
C 5.314733 -0.504880 -0.581240
C -1.656266 2.038749 -1.625825
C -2.555170 3.146033 -1.028079
C -0.424635 2.695240 -2.284076
C -2.426058 1.226871 -2.689931
Si 1.860541 -1.850713 -1.388613
C 2.977495 -2.174372 -2.903219
C 2.360493 -3.081078 -0.014724
C 0.048711 -2.186428 -1.880071
C 0.382465 -1.210474 2.905142
C -2.033258 -0.580686 3.109791
C 4.500317 2.353327 0.323819
C 3.832344 -0.119733 2.114276
H -2.706523 -2.030127 -1.171070
H -5.096631 -2.702493 -1.392426
H -6.889195 -1.314992 -0.338487
H -6.275947 0.741381 0.945761
H -3.878824 1.401318 1.168672
H 0.325341 -1.894671 3.765602
H 1.189401 -1.545795 2.239740
H 0.627516 -0.199952 3.263236
H -1.432500 -3.258064 2.695927
H -2.345366 -2.667105 1.282535
H -0.612573 -3.085005 1.117093
H -2.043620 -1.136997 4.061087
H -1.774487 0.469100 3.316783

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H -0.767563 3.389278 -3.067073
H 0.156326 3.258715 -1.538192
H 0.231230 1.937331 -2.735722
H -2.824110 3.866326 -1.817723
H -3.482730 2.722690 -0.617917
H -2.014772 3.678704 -0.231046
H -2.648177 1.887885 -3.542381
H -1.811786 0.387200 -3.051651
H -3.375199 0.832852 -2.303989
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H 3.039588 0.412797 2.662860
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H 2.349975 -4.111367 -0.414273
H 3.376119 -2.882459 0.364528
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29-PH
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C 4.002013 0.220413 -1.148364
C 0.360202 0.038358 -0.104111
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N -0.423504 -1.061597 -0.071304
Si -1.960130 -0.034500 0.053662
Cl -2.856538 0.120218 -1.859899
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C -1.379912 -3.230638 -0.575476
C 1.063703 -2.839250 -1.037699
C 0.225853 -2.964633 1.355578
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C 0.803262 3.112108 -0.933799
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H 1.896188 -0.322312 2.089410

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H 0.466656 3.787281 1.762196
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H -2.229125 -3.008650 0.089103
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H 0.375707 -4.056074 1.376122
H 1.147608 -2.480107 1.710037
H -0.601592 -2.706870 2.033684
H 1.148527 -3.933983 -1.119842
H 0.870769 -2.428321 -2.040836
H 2.020844 -2.448410 -0.668869
P -3.049052 -0.277779 1.852663
H -4.152308 0.490923 1.340285

30-PH
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C -4.351625 -0.032392 0.890943
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C -2.130164 -0.041821 -0.099234
C -2.702487 -0.047065 -1.385697
C -4.096629 -0.050377 -1.528784
C -0.653304 -0.010458 0.061542
N 0.150923 -1.066430 0.286565
C -0.122709 -2.524837 0.279548
C 1.246927 -3.227931 0.383489
N 0.126351 1.084448 0.029218
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Br 2.806418 -0.088286 -1.460540
C -0.212439 2.525723 0.139326
C 1.086480 3.297509 -0.176630
C -1.307525 2.939310 -0.866855
C -0.664875 2.828284 1.586195
C -0.989824 -2.901581 1.501815
C -0.817876 -2.949306 -1.032595
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H -4.537417 -0.056671 -2.527419
H -6.008542 -0.039106 -0.506189
H -4.989922 -0.024253 1.776405
H -2.504862 -0.032137 2.033034
H 1.090915 -4.317277 0.411278
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H -0.220518 -2.628219 -1.899996
H -1.110916 -3.996089 1.539653
H -0.500067 -2.569549 2.430306
H -1.987479 -2.444518 1.435808
H 0.896781 4.377731 -0.081480

H 1.885510 3.014508 0.526045
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P 2.776290 0.256299 2.260925
H 1.531206 0.211481 2.999412

31-PH

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C	3.556822	0.079058	0.733413
C	4.910862	-0.294508	0.738040
C	5.370110	-1.363262	-0.042686
C	4.473675	-2.057582	-0.859398
N	1.253880	-0.356962	0.025674
Si	-0.200049	0.426850	-1.101016
N	-0.547871	2.066038	-0.564933
Si	0.740111	3.308925	-0.674185
C	2.320824	2.606522	-1.463295
C	3.075028	1.241203	1.602554
C	4.066412	2.423880	1.608209
C	2.190491	-2.522742	-1.826727
C	2.129889	-4.014454	-1.427478
C	0.369372	-1.264189	0.496602
N	0.607188	-2.371769	1.245088
C	1.818327	-2.600184	2.039100
N	-0.860953	-0.916103	0.026208
C	-2.090177	-1.213144	0.691422
C	-2.297894	-0.763977	2.022091
C	-3.520900	-1.074340	2.643322
C	-4.524339	-1.774800	1.963845
C	-4.303627	-2.197145	0.648230
C	-3.084938	-1.943793	-0.005452
C	-1.262873	0.051144	2.798977
C	-0.715032	-0.761921	3.993869
C	-2.868825	-2.475621	-1.421682
C	-3.792021	-1.769353	-2.440264
C	-0.334023	-3.500845	1.238919
C	-3.083081	-4.007098	-1.489068
C	-1.839611	1.397657	3.290058
Si	-2.227666	2.700175	-0.713403
C	-2.647492	3.201033	-2.499884
C	-3.579522	1.472867	-0.204156
C	-2.423380	4.204610	0.449044
C	2.762584	0.810655	3.055152
C	2.639422	-2.379098	-3.297756
C	0.296675	4.753487	-1.841259
C	1.030788	4.064079	1.053938
H	-5.083652	-2.745009	0.116018
H	-5.474216	-1.989924	2.458257
H	-3.692143	-0.740570	3.668767
H	4.833057	-2.877325	-1.484691

H	5.615074	0.256495	1.363032
H	-1.833890	-2.258414	-1.720721
H	-3.672489	-2.230907	-3.433473
H	-4.849275	-1.856338	-2.137860
H	-3.523899	-0.708097	-2.534611
H	-2.849125	-4.368715	-2.503236
H	-2.444149	-4.547837	-0.772003
H	-4.130295	-4.270754	-1.268128
H	-0.426431	0.300147	2.134242
H	0.069811	-0.193727	4.519298
H	-1.521408	-0.978943	4.713429
H	-0.289704	-1.719590	3.659781
H	-1.054333	1.972373	3.808300
H	-2.205531	1.993515	2.443563
H	-2.672544	1.244059	3.995120
H	1.175801	-2.109852	-1.772984
H	1.946243	-2.930938	-3.952201
H	2.620714	-1.322779	-3.599399
H	3.655146	-2.784127	-3.442836
H	1.434965	-4.552109	-2.093110
H	3.121474	-4.488091	-1.517828
H	1.784119	-4.141396	-0.391203
H	2.133243	1.594673	1.171099
H	3.606345	3.284825	2.115704
H	4.992134	2.171888	2.150792
H	4.334012	2.720770	0.583932
H	2.514486	1.697885	3.661615
H	1.900942	0.129273	3.097620
H	3.631954	0.312426	3.515824
H	1.513532	-2.977366	3.028948
H	2.467669	-3.344550	1.550419
H	2.381250	-1.677493	2.170880
H	0.253253	-4.428765	1.315961
H	-1.043884	-3.444144	2.079667
H	-0.890824	-3.517362	0.297837
H	1.132060	5.476716	-1.821119
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H	-0.620285	5.298227	-1.575784
H	1.971579	4.639560	1.082676
H	0.209232	4.754309	1.305229
H	1.073217	3.303177	1.848406
H	3.100146	3.388754	-1.436777
H	2.738888	1.706270	-1.000628
H	2.122694	2.366740	-2.520820
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32-PH
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33-PH
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C 3.343227 -3.153293 -4.187147

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H -2.137169 3.437209 -1.393475
H -3.214214 -2.866161 1.294766
H -3.667511 -4.154262 0.147320
H -4.780916 -2.794920 0.434640
H -8.625661 -1.041897 1.928215
H -4.403728 -0.245542 2.442624
H -8.357338 -0.830561 -0.547537
H -4.215384 2.479577 -2.553848
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H -5.629980 1.980203 -1.573531
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H -1.347315 1.718057 3.773822
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H 0.187428 -0.444195 -3.412005

38-PH

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Fe -0.040311 -0.372945 2.150801
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39-PH
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40-PH
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41-PH

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C	-5.471083	-1.293711	-0.999510
C	-5.895012	-0.266645	-1.860085
C	-5.063569	0.841504	-2.091098
C	-2.056418	-0.030057	0.052192
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C	-2.472133	1.733276	1.817531
C	-2.890707	3.043706	1.120519
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N	1.662782	-1.024688	0.665296
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C	3.408658	0.361191	-0.511880
C	4.350323	1.227943	0.077480
C	5.594635	1.434136	-0.533126
C	5.902772	0.789200	-1.742924
C	4.964481	-0.070476	-2.336780
C	3.724285	-0.289990	-1.720524
C	3.644031	-1.710427	2.044602
C	0.684199	1.948970	-1.941206
C	-1.422926	-1.637841	-2.505078
C	-3.685036	1.004044	2.429238
H	0.286146	-1.949016	-1.237239
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H	-3.158060	1.779349	-1.641029
H	-5.387268	1.638764	-2.763283
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H	-6.117808	-2.153129	-0.811488
H	-3.882349	-2.003931	0.298545
H	-1.025482	-2.362121	-3.234185
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H	-1.159360	-0.623700	-2.842825
H	-0.883040	-4.115691	-1.295758
H	-0.800204	-3.508673	0.391038
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H	4.419358	-1.220952	1.435888
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H	6.870891	0.955069	-2.219858
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H	4.102101	1.721267	1.017642
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H	-1.107937	0.112791	3.681178

42-PH

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C	4.425564	-0.649499	-2.850215
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C	2.707984	2.045501	0.912936
C	2.401456	2.559533	2.330281
C	-0.978524	3.462860	0.205241
C	0.770747	-1.892914	-1.209719
C	0.515748	-0.995348	-2.438847
C	1.684613	-3.076439	-1.559596
C	2.596260	3.201067	-0.107819
C	4.448186	-1.240596	0.317456
C	4.899954	-0.435289	1.559428
C	3.904305	-2.606574	0.777055
C	5.276440	1.196489	-1.360007
C	-5.295285	-1.419879	-0.754918
H	-1.339314	-2.439543	2.108454
H	0.263931	2.111160	-0.883790
H	-2.710094	-4.213465	1.413330
H	-3.642783	-3.252152	0.253165

H	-1.923867	-3.634713	-0.079285
H	-3.591678	-2.399694	3.105701
H	-2.837428	-0.780580	3.059407
H	-4.135840	-1.201419	1.902087
H	-0.574401	4.340018	-0.327264
H	-2.034380	3.668053	0.440839
H	-0.436383	3.337836	1.153055
H	-1.002250	3.108395	-2.603545
H	-1.502784	1.397773	-2.590260
H	-2.568570	2.653214	-1.911089
H	-0.197160	-2.306760	-0.897566
H	0.087526	-1.580942	-3.269462
H	-0.184621	-0.193320	-2.170385
H	1.454890	-0.536485	-2.786698
H	1.241886	-3.627494	-2.406229
H	2.686821	-2.734929	-1.847310
H	1.774830	-3.762509	-0.706419
H	3.743315	1.685879	0.894354
H	2.907381	3.526097	2.489347
H	1.318559	2.689204	2.473021
H	2.751590	1.851144	3.093056
H	3.365071	3.960096	0.112128
H	2.746850	2.842734	-1.137241
H	1.611890	3.684415	-0.044458
H	3.237888	0.951108	-2.029486
H	4.815058	-0.079311	-3.709625
H	5.206675	-1.359003	-2.532029
H	3.547574	-1.225235	-3.173911
H	5.611214	1.703610	-2.279105
H	5.042325	1.964052	-0.611956
H	6.115521	0.588003	-0.989113
H	5.331902	-1.424836	-0.313522
H	5.594274	-1.043331	2.162010
H	5.415921	0.493570	1.278674
H	4.030456	-0.187581	2.187981
H	4.604891	-3.041306	1.507422
H	2.922807	-2.494442	1.259010
H	3.810417	-3.301207	-0.065143
H	-3.202456	-1.734118	-1.083174
H	-3.343191	2.223306	0.032294
H	-5.428017	2.943595	-0.927611
H	-4.523422	2.080506	-2.198679
H	-5.901037	1.297509	-1.387402
H	-5.354110	2.276197	1.451625
H	-5.652089	0.543963	1.138942
H	-4.182936	1.052864	2.020897
H	-5.550355	-2.327389	-1.325673
H	-5.292826	-1.678121	0.310816
H	-6.090069	-0.682877	-0.934030
H	-4.118798	-1.580832	-3.283202
H	-4.712667	0.077442	-3.034598
H	-2.954485	-0.243304	-3.071681
H	1.405715	0.288239	3.395214

43-PH

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Si -4.177040 -1.233113 -0.167370
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P -2.136800 0.978299 1.086740
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C -3.356959 2.385865 1.026615
P -1.291225 -0.274170 -1.214961
C -1.825920 0.315044 -2.899329
Si -0.005648 1.380560 -0.109162
P 1.303490 -0.044809 1.252093
C 0.543384 -1.616100 1.926993
C 2.556484 -0.334474 0.066217
Si 4.191215 -1.169511 0.352888
C 5.468012 0.005938 1.162107
C 1.824041 0.845410 2.803324
C -0.509674 -1.934641 -1.589589
C -3.933300 -2.960792 -0.955240
C -5.001998 -1.445575 1.544319
P 2.132131 0.778022 -1.243708
C 2.261735 -0.034713 -2.923681
C 3.370814 2.158317 -1.437868
C 3.986221 -2.672333 1.519602
C 4.933617 -1.760510 -1.306190
H -4.901614 -3.480808 -1.060353
H -3.488541 -2.892728 -1.963431
H -3.274752 -3.600254 -0.342725
H -6.374677 -0.789825 -1.368988
H -5.591592 0.738152 -0.885791
H -4.998697 -0.150596 -2.304218
H -5.938213 -2.023854 1.454744
H -4.343755 -1.976086 2.252528
H -5.262942 -0.471823 1.994258
H 5.876769 -2.310040 -1.141032
H 4.242969 -2.426979 -1.849298
H 5.165274 -0.908027 -1.967927
H 6.442337 -0.490768 1.319509
H 5.643163 0.895765 0.533210
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H 4.960072 -3.156778 1.708832
H 3.575276 -2.374265 2.500163
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H -2.223343 1.335761 -2.798852
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H -2.610074 -0.345664 -3.303262
H -1.183449 -2.730385 -1.240440
H -0.332393 -2.057938 -2.669555
H 0.451809 -2.007607 -1.057158
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H -3.318424 0.236634 3.135980
H -1.651270 -0.402326 3.073168
H -3.051855 3.180423 1.725797
H -3.363664 2.801194 0.009377
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H 3.098623 2.805900 -2.286921
H 3.371552 2.762080 -0.519341
H 4.380375 1.747454 -1.606056
H 1.912976 0.665922 -3.700467

H 3.302706 -0.318594 -3.143901
H 1.638558 -0.938867 -2.943931
H 0.284042 -1.505151 2.991439
H -0.369932 -1.851531 1.359671
H 1.266383 -2.437149 1.816119
H 2.599358 0.271352 3.336477
H 2.221258 1.832344 2.524498
H 0.956105 0.985413 3.468132
P -0.139760 3.533758 -0.201380
H 1.066674 3.696358 -0.971792

44-PH
C 1.098574 3.204734 0.000000
C -0.377848 2.774378 0.000000
C -1.060989 3.333621 1.270157
N -0.480474 1.284972 0.000000
C -1.761054 0.695064 0.000000
C -1.763688 -0.661053 0.000000
N -0.487673 -1.253408 0.000000
C -0.379272 -2.743409 0.000000
C -1.060989 -3.304003 -1.269961
Si 0.730656 0.009435 0.000000
C -1.060989 3.333621 -1.270157
C 1.101020 -3.163022 0.000000
C -1.060989 -3.304003 1.269961
H -2.644555 1.326098 0.000000
H -2.650115 -1.288050 0.000000
H -0.979686 4.432074 1.281478
H -2.128165 3.067741 1.303337
H -0.572287 2.931339 2.170703
H 1.150230 4.304035 0.000000
H 1.619371 2.832067 0.894752
H 1.619371 2.832067 -0.894752
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H -0.572287 2.931339 -2.170703
H -2.128165 3.067741 -1.303337
H 1.161008 -4.261927 0.000000
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H -2.129820 -3.043539 1.302152
P 2.847707 -0.194834 0.000000
H 3.009081 1.229584 0.000000

45-PH
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C 2.674531 -0.015331 -0.351819
C 3.322129 -1.210240 0.034989
C 4.715355 -1.183928 0.214272
C 5.466204 -0.011827 0.019379
C 4.790307 1.159050 -0.365610
N 1.253155 -0.015816 -0.539762

Si 0.001457 -0.034096 0.680247
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C 6.965521 -0.005662 0.246195
C 2.682606 2.467863 -0.912258
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C -3.329346 1.213609 0.141533
C -4.723874 1.160749 0.309252
C -5.463399 0.004186 0.011057
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C -3.382987 -1.121876 -0.643686
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C -6.964116 -0.035699 0.224900
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H -7.212605 -0.463468 1.212598
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H 2.182166 2.397096 -1.891889
H 1.893358 2.694990 -0.175533
H 3.388338 3.311452 -0.941946
H 7.413501 -0.976481 -0.019896
H 7.457149 0.778889 -0.350435
H 7.205200 0.186461 1.307269
P -0.106941 -0.176562 2.780841
H 1.334775 -0.199177 2.788845

46-PH
C -3.351897 -1.234822 -0.230916
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C -0.681223 0.004974 -1.803156
C 0.679276 0.004969 -1.801534
N 1.246901 0.001526 -0.509182
Si -0.000598 -0.001574 0.707329
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C 2.670203 0.000901 -0.322079
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C 4.744322 1.214515 -0.055174
C 5.438769 -0.000341 0.027342
C 4.743719 -1.214579 -0.059057
C 3.348289 -1.234844 -0.232539
C 2.583568 2.541578 -0.293904
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H 1.338230 0.007208 -2.665913
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H 1.929246 2.657067 0.587479
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H -1.337134 -0.007565 2.814438

47-PH
C 3.117396 1.314430 -0.146255
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C 0.681810 -0.107899 -1.824261
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C 2.650190 3.541450 -1.279884
C -2.655031 -0.022096 -0.319129
C -3.138560 1.301094 -0.165965
C -4.507219 1.473813 0.107120
C -5.364805 0.372760 0.223204
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C -3.504510 -1.149316 -0.218306
C -2.215646 2.516637 -0.246269
C -2.025379 3.144245 1.154590

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H -2.014100 4.400387 -1.327774
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48-PH
C -3.177342 1.125506 -0.069885
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C 3.191764 1.190643 0.075229
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H -2.949421 -0.638743 -2.165486
H -3.095611 -2.158358 -1.232544
H 4.288217 1.261859 0.141183
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H 2.756460 1.685541 0.956235
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49-PH
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C -3.519407 -0.695425 -1.371168
C -0.820731 -1.611534 -0.625447
C 0.626093 -1.720987 -0.091411
C 0.646664 -2.211737 1.371516
P 0.252747 2.863007 0.374754
C 3.066140 0.918824 -1.260310
C 3.111604 0.348998 1.203605
H -0.826832 -1.707443 -1.727237
H -4.413641 -0.867275 1.243590
H -3.072231 -2.023982 1.063536
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H -4.310054 1.399528 0.190758
H -2.753709 1.736112 0.998840
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H -3.165177 -0.139936 -2.253692
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50-PH
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Si -0.298021 -1.092930 -0.341794
N 1.134946 -0.260753 0.183033
C 2.371859 -0.962460 0.684954
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C -3.367718 0.133691 1.892419
C -0.696740 1.049959 1.101140
C 0.759658 1.128740 0.561574
C 0.942552 2.183019 -0.599219
C 0.658391 3.598057 -0.039048
C 2.398643 2.158878 -1.106554
C 0.008718 1.913729 -1.797888
C 1.971164 -2.056923 1.708459
C 3.097409 -1.617350 -0.512172
H -0.678044 0.797482 2.177636
H -4.564206 1.290724 -0.294237
H -3.068979 2.206723 0.011653
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54-PH
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H -1.223848 -3.208256 3.922470
H -2.438736 -1.776804 2.316939
H -5.325890 -0.842970 -1.485393
H -5.973526 -3.029247 -2.493436
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H -1.655038 -2.617220 -0.042298
H -2.366423 1.164038 2.628762
H -6.133194 1.001887 4.737691
H -7.174554 -0.142667 2.783827
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H 4.445610 0.399653 -2.624334
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H 2.626445 2.694925 0.558750
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H 4.778423 1.537842 1.499122
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H 2.642685 -4.271413 -4.009684
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H -5.263914 5.408804 -1.813635
H -4.243631 1.998760 5.836213
H -2.694649 1.222404 5.401590
H -3.095759 2.818648 4.741166
H 6.751744 2.267466 2.755759
H 6.314457 1.541626 4.319113
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H 0.102590 -4.484241 -3.232051
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H -0.023984 -3.015254 -4.222520
P 0.192887 2.688990 -1.668686
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58-PH
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Si -2.422371 -1.643206 -0.494692
C -3.265356 -1.742126 -2.206913
Si -0.009891 -0.033341 0.861142
C 1.457630 -0.040002 -0.353152
Si 2.746333 -1.434029 0.057960
C 3.944001 -0.892921 1.440724
C -0.710546 0.361729 -1.692754
C 0.691210 -0.313385 -1.709967
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H 4.307213 -1.060216 -1.927785
H 4.651944 -1.715204 1.645133
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H 1.313759 -0.258019 3.068177

59-PH
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C 4.289539 -0.709815 -0.046676
C 5.514131 -1.366745 -0.287504
C 6.670986 -0.632184 -0.593355
C 6.617098 0.770793 -0.657672
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C 2.331922 -3.108217 -0.623854
Si 2.527193 1.446111 0.275383
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C 1.419127 -0.104951 -0.063081

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C -3.109963 2.421323 -2.154181
C -0.291922 0.631757 -1.832453
C 1.007821 -0.176125 -1.587506
Si -2.416218 -1.287509 -1.079395
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C -4.006152 -0.825634 -0.157174
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C -6.286316 0.109130 1.222609
C -6.156394 -1.257292 0.921278
C -5.022058 -1.720795 0.236569
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60-PH

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61-PH
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C 1.811934 -4.998813 -1.122614
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62-PH
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63-PH
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64-PH
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65-PH

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C	2.730882	-3.561059	-1.095735
C	3.137073	3.185969	-2.021121
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H	4.298337	-3.529355	1.242214
H	3.216173	-2.500348	2.216949
H	2.166156	-4.464840	-0.810824
H	2.260714	-3.119758	-1.987563
H	3.761540	-3.865504	-1.343055
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66-PH

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C	2.081777	-1.206035	3.354715
C	2.299759	-1.899204	1.961044
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67-PH

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H -1.618169 -2.335992 2.009662
H -2.939997 -3.456622 1.569941
H -1.543910 -4.343934 -1.182449
H -3.288144 -4.081156 -0.951362
H -2.402998 -3.153117 -2.200003
H 1.045373 -2.122994 0.690903
H 1.936904 -4.133412 1.835799
H 3.607023 -3.663292 1.417793
H 2.652465 -2.649250 2.533228
H 1.259508 -4.217238 -0.610613
H 1.484065 -2.780423 -1.659177
H 2.898882 -3.751430 -1.142470
H 1.587443 2.556836 0.212434
H 2.936988 4.472343 1.078628
H 3.244503 2.993978 2.039489
H 4.440075 3.541369 0.834198
H 2.310364 4.307789 -1.381850
H 3.809870 3.407316 -1.737617
H 2.221806 2.708883 -2.184558
P 0.121304 0.120623 -2.023766
H -1.302844 0.071781 -2.182922

83-PH
C 2.229987 -1.693757 0.857666
C 1.527938 -0.731076 0.109703
C 1.999464 -0.356398 -1.166303
C 3.160998 -0.946289 -1.686986
C 3.856411 -1.910658 -0.938610
C 3.389780 -2.283373 0.332270
P -0.029883 -0.018021 0.831174
C -1.398962 -0.969108 0.047368
C -1.200899 -1.686173 -1.149886
C -2.274443 -2.357362 -1.753331
C -3.549959 -2.320106 -1.168384
C -3.750792 -1.609648 0.025838
C -2.682600 -0.933011 0.632907
C -0.084196 1.668895 0.081907
C 1.052041 2.500565 0.171504
C 1.002302 3.815300 -0.311532
C -0.178115 4.309304 -0.891334
C -1.309703 3.483503 -0.984191
C -1.266862 2.168444 -0.497558
H 1.974770 2.116978 0.611725
H 1.886221 4.452621 -0.238272
H -0.215023 5.333213 -1.269307
H -2.228455 3.861616 -1.437831
H -2.148996 1.530330 -0.569368
H -0.210723 -1.727914 -1.604302
H -2.111242 -2.913768 -2.678786
H -4.383538 -2.844939 -1.640124
H -4.739804 -1.580895 0.487922
H -2.833950 -0.379015 1.561168
H 1.464135 0.398817 -1.744124
H 3.525045 -0.649787 -2.673297
H 4.762932 -2.365716 -1.343855
H 3.932345 -3.028857 0.917812
H 1.863069 -1.958302 1.853328
P -0.263291 -0.118852 2.929219
H 0.726485 0.914405 3.095126

84-PH
C 1.848191 -0.919919 -1.292496
C 1.634179 -0.899921 0.239288
C 2.862004 -0.276819 0.947154
C 4.144622 -1.057686 0.585377
C 4.358949 -1.121496 -0.940852
C 3.123504 -1.715248 -1.647914
P 0.023141 -0.103958 0.764683
C 0.075571 1.664746 0.080946
C -0.686433 2.653713 0.994550
C -0.482333 4.105492 0.513380
C -0.913470 4.278912 -0.957267
C -0.176448 3.277453 -1.869075
C -0.389097 1.824197 -1.387620
C -1.298188 -0.971544 -0.260556
C -2.701756 -0.474980 0.160172
C -3.812046 -1.188034 -0.639865

C -3.707475 -2.718300 -0.487573
C -2.312588 -3.215109 -0.916844
C -1.192397 -2.507364 -0.123113
H -1.126777 -0.697333 -1.315211
H -2.833518 -0.678835 1.236452
H -2.779335 0.615904 0.024560
H -4.799776 -0.833329 -0.301092
H -3.719997 -0.921796 -1.709138
H -3.876242 -2.987483 0.570435
H -4.490890 -3.217469 -1.081856
H -2.232181 -4.305981 -0.776591
H -2.174554 -3.015198 -1.995579
H -1.263985 -2.769433 0.946405
H -0.210294 -2.856229 -0.480866
H 1.148000 1.928739 0.134354
H -1.763821 2.410968 0.974040
H -0.346015 2.530429 2.033610
H -1.044807 4.796791 1.162673
H 0.587382 4.366736 0.610832
H -2.001699 4.102109 -1.037244
H -0.726427 5.311993 -1.294501
H -0.521603 3.377973 -2.911870
H 0.905207 3.504549 -1.860779
H -1.462911 1.581212 -1.455688
H 0.141735 1.127064 -2.052744
H 1.541108 -1.942850 0.588347
H 2.973077 0.773696 0.623645
H 2.708502 -0.267636 2.035891
H 5.014287 -0.590799 1.076399
H 4.059611 -2.085027 0.983154
H 4.533170 -0.099208 -1.324018
H 5.257328 -1.714936 -1.178271
H 3.268745 -1.718824 -2.741004
H 2.990512 -2.765970 -1.332637
H 1.966892 0.115850 -1.653484
H 0.974996 -1.351315 -1.806509
P -0.127568 -0.331558 2.864291
H -1.378054 0.379829 2.887526

2.4. Structures with connected =P-H units (transition states)

1-PH(TS)
C -3.162133 -2.226565 1.301088
C -2.754962 -1.745284 0.029791
C -2.583327 -2.605476 -1.081805
C -2.805274 -3.981884 -0.893984
C -3.185050 -4.482917 0.356059
C -3.367480 -3.611497 1.436789
N -2.520487 -0.335425 -0.136112
C -3.555640 0.559576 -0.425632
C -3.066712 1.831601 -0.412099
N -1.689229 1.797736 -0.133295
C -0.931164 3.007110 -0.001062
C -0.364757 3.328756 1.264905
C 0.419567 4.492486 1.357968
C 0.596888 5.342665 0.258934

C -0.017809 5.039367 -0.958002
C -0.778819 3.866371 -1.119127
C -0.696282 2.514684 2.517915
C -2.131059 2.853810 2.991959
C -1.416850 3.583398 -2.479750
C -0.410835 3.710933 -3.645981
C -2.255690 -2.045381 -2.462830
C -1.330380 -2.953815 -3.297315
C -3.434607 -1.273952 2.464911
C -4.907105 -0.793259 2.427498
B -1.291404 0.409842 0.048497
Si 0.380543 -0.443553 0.774275
P 0.424406 -1.436976 2.662923
N 1.749908 -0.407852 -0.286612
Si 1.993734 0.524721 -1.827345
C 3.477065 -0.224912 -2.740041
C 2.903562 -1.207104 0.114589
C 3.925308 -0.643071 0.915907
C 5.028740 -1.447108 1.256472
C 5.123873 -2.772735 0.824754
C 4.105319 -3.314037 0.032377
C 2.988602 -2.548116 -0.342189
C 3.880985 0.793515 1.429156
C 5.088590 1.607608 0.908331
C 1.881000 -3.188094 -1.177854
C 0.970719 -4.060740 -0.281738
C 0.459458 0.350287 -2.926601
C 2.364345 2.335904 -1.414824
C 2.416979 -4.024652 -2.360489
C 3.843768 0.834889 2.974299
C 0.309771 2.680941 3.671751
C -2.612849 4.535902 -2.722573
C -3.563532 -1.757854 -3.238957
C -3.130916 -1.882298 3.848785
H 3.658934 0.343100 -3.669649
H 4.393982 -0.191325 -2.131617
H 3.298619 -1.276113 -3.012852
H 0.632172 0.852871 -3.893374
H 0.257845 -0.711771 -3.134417
H -0.442038 0.789051 -2.475300
H 2.364868 2.951544 -2.330098
H 1.623571 2.767896 -0.727892
H 3.355665 2.434393 -0.949210
H 4.174546 -4.351354 -0.299614
H 5.985223 -3.382884 1.105307
H 5.818198 -1.020912 1.879218
H 1.261351 -2.382933 -1.597365
H 0.130785 -4.473032 -0.863145
H 1.552956 -4.895965 0.140833
H 0.563139 -3.483303 0.560730
H 1.577530 -4.356245 -2.992929
H 3.118638 -3.447817 -2.983446
H 2.940234 -4.926546 -2.005281
H 2.962655 1.268433 1.057592
H 4.991912 2.666177 1.201679
H 6.027770 1.219687 1.335223

H 5.172924 1.552591 -0.188414
H 3.748018 1.876870 3.323742
H 2.998933 0.246073 3.359117
H 4.773933 0.418724 3.394782
H -4.563379 0.208777 -0.621006
H -3.579726 2.772979 -0.572326
H 0.880174 4.750290 2.311523
H 1.205404 6.244148 0.357621
H 0.108587 5.708427 -1.810701
H -0.705401 1.444609 2.272319
H -2.390099 2.237082 3.868258
H -2.200185 3.916954 3.277460
H -2.864985 2.653407 2.197292
H 0.073086 1.952964 4.462396
H 1.343124 2.500770 3.336279
H 0.257503 3.689819 4.114278
H -1.798781 2.553460 -2.483200
H -3.093416 4.308443 -3.688459
H -3.369729 4.451152 -1.927640
H -2.267684 5.582585 -2.746295
H -0.894910 3.407073 -4.588334
H -0.067431 4.750923 -3.765760
H 0.468056 3.074205 -3.481870
H -3.666420 -4.012836 2.405368
H -3.343260 -5.555595 0.488606
H -2.679778 -4.664973 -1.735377
H -1.743537 -1.085769 -2.321596
H -3.335039 -1.328480 -4.229078
H -4.135072 -2.689330 -3.386110
H -4.197568 -1.045605 -2.689485
H -1.035194 -2.431800 -4.221842
H -0.421589 -3.220138 -2.739104
H -1.838199 -3.886453 -3.592390
H -2.778141 -0.400894 2.338516
H -5.092544 -0.086538 3.253729
H -5.149966 -0.288152 1.481924
H -5.589002 -1.651899 2.548313
H -3.219178 -1.095472 4.615351
H -3.851533 -2.676853 4.107016
H -2.109744 -2.286555 3.880748
H 0.845061 -0.174376 3.220440

2-PH(TS)
C -1.913216 2.821204 0.993543
Si -2.794234 1.314489 0.223112
C -1.503518 0.037655 -0.431611
Si -2.206823 -1.724492 -0.783699
C -0.972611 -2.601373 -1.947206
C -3.783701 1.931663 -1.287552
C -3.935048 0.535635 1.524662
Si 0.014921 -0.099879 0.658966
P 0.024364 -0.027759 2.794625
C 1.522663 -0.095987 -0.455359
Si 2.926249 -1.271120 0.153266
C 2.171521 -2.895494 0.810096
Si 2.066999 1.731806 -0.764842

C 2.103870 2.717487 0.860195
C 3.782996 1.806791 -1.589729
C 0.806563 2.510482 -1.969171
C -2.385705 -2.734179 0.815860
C -3.890915 -1.619313 -1.668596
C 4.017494 -1.705771 -1.350483
C 3.941954 -0.449318 1.529858
H -1.157548 0.382618 -1.426322
H 1.183687 -0.443813 -1.451836
H -4.642095 1.286073 1.918782
H -4.526770 -0.302794 1.121566
H -3.329556 0.161577 2.366811
H -4.501477 2.715047 -0.987147
H -3.112465 2.373689 -2.044765
H -4.351383 1.122926 -1.773589
H -2.652570 3.585747 1.290493
H -1.357138 2.528471 1.899255
H -1.209446 3.302189 0.292724
H -4.240245 -2.633043 -1.932104
H -4.662129 -1.152578 -1.035313
H -3.822259 -1.034007 -2.600554
H -2.876382 -3.700986 0.606797
H -1.406691 -2.950250 1.275697
H -2.986184 -2.200945 1.568804
H -1.342131 -3.600665 -2.236042
H -0.815426 -2.025145 -2.875813
H 0.012669 -2.738157 -1.470783
H 4.040672 2.856795 -1.814511
H 4.575223 1.399071 -0.942227
H 3.802133 1.246391 -2.539032
H 2.551680 3.712555 0.691144
H 1.094752 2.876307 1.275614
H 2.695147 2.201063 1.632368
H 1.087833 3.549442 -2.214365
H 0.762486 1.947597 -2.918080
H -0.211496 2.532640 -1.548376
H 2.967568 -3.607246 1.090960
H 1.558782 -2.708174 1.706795
H 1.537397 -3.394238 0.056292
H 4.756253 -2.480040 -1.078626
H 3.409148 -2.108802 -2.179139
H 4.569848 -0.833925 -1.733708
H 4.703664 -1.143554 1.925220
H 4.463947 0.457508 1.181820
H 3.271356 -0.164339 2.357690
H -0.079961 -1.466777 2.801850

3-PH(TS)
C -3.437717 2.133621 0.038346
Si -2.861258 0.516038 -0.790240
C -2.532955 0.896349 -2.621818
C -4.272795 -0.750800 -0.676770
N -1.364261 -0.066988 0.031556
Si -1.542580 -0.853893 1.643922
C -2.178204 -2.630542 1.403184
Si 0.030873 -0.520176 -0.913425

P 0.084460 -1.878623 -2.562254
N 1.439320 0.152323 -0.161895
Si 1.485613 1.917334 0.168305
C 0.324939 2.821442 -1.037978
Si 2.920042 -0.867265 0.003107
C 2.472905 -2.717778 -0.020039
C 4.171050 -0.541585 -1.383446
C 3.668384 -0.486013 1.714945
C 0.102094 -1.016291 2.579697
C -2.753868 0.126528 2.733161
C 1.004860 2.377987 1.946922
C 3.228879 2.593486 -0.196495
H -1.647852 1.532784 -2.784104
H -2.400467 -0.026270 -3.205593
H -3.405167 1.442264 -3.023896
H -2.647209 2.900875 0.065874
H -4.280293 2.550113 -0.542099
H -3.788022 1.981728 1.069810
H -3.982559 -1.706848 -1.141563
H -4.575497 -0.954208 0.362936
H -5.159794 -0.367965 -1.211598
H -0.127097 -1.407864 3.587208
H 0.786781 -1.730528 2.100968
H 0.639075 -0.067610 2.692874
H -2.781794 -0.334398 3.736043
H -2.445071 1.177587 2.853954
H -3.781732 0.119361 2.337615
H -2.216620 -3.162848 2.370261
H -3.181425 -2.669963 0.953546
H -1.500934 -3.193089 0.737039
H 1.065217 3.473401 2.074482
H -0.026172 2.067545 2.179174
H 1.676174 1.918978 2.691125
H 3.237047 3.676334 0.020314
H 4.031828 2.131283 0.396623
H 3.482147 2.465886 -1.261215
H 0.465439 3.911769 -0.934298
H 0.551331 2.559665 -2.086065
H -0.734824 2.605162 -0.850810
H 4.995144 -1.274711 -1.328406
H 3.676534 -0.665853 -2.360922
H 4.612325 0.465818 -1.340973
H 4.642651 -0.995261 1.818808
H 3.835046 0.587348 1.894927
H 3.007880 -0.858238 2.514801
H 3.288070 -3.286686 0.462405
H 1.545138 -2.961147 0.525009
H 2.355683 -3.082130 -1.051239
H -0.246374 -0.767247 -3.418469

4-PH(TS)
C 1.074892 3.235644 0.779643
C 0.040908 3.117253 -0.190954
C 0.380774 3.075895 -1.574173
C 1.731805 3.049580 -1.942186

C 2.767613 3.070500 -0.990804
C 2.417875 3.178830 0.361089
C -1.399055 3.129119 0.220464
C -2.255546 2.002358 0.056577
C -3.623843 2.081564 0.408160
C -4.118178 3.284234 0.951489
C -3.283424 4.390882 1.140987
C -1.936803 4.309727 0.768041
C -4.605584 0.970459 0.189326
C -4.865770 0.031370 1.214493
C -5.887896 -0.914888 1.021962
C -6.654310 -0.950578 -0.153641
C -6.369168 -0.015783 -1.163781
C -5.353518 0.942843 -1.012968
C -4.064529 0.046123 2.497635
C -5.068930 1.936711 -2.123534
C -7.727233 -2.001751 -0.353079
S -1.642450 0.480513 -0.709231
Si -0.005776 -0.017399 0.621235
P -0.050793 -0.271083 2.732569
C -0.674996 3.094681 -2.662751
C 4.211343 2.975612 -1.427048
C 0.791836 3.507255 2.245384
S 1.646959 -0.462698 -0.701843
C 2.266482 -1.995920 0.029044
C 1.412939 -3.126273 0.174700
C 1.957070 -4.317797 0.690043
C 3.306611 -4.404195 1.051295
C 4.137417 -3.290875 0.884653
C 3.636202 -2.077443 0.373126
C -0.032195 -3.104127 -0.217269
C -0.392028 -3.047391 -1.595234
C -1.748218 -3.022056 -1.942468
C -2.768930 -3.059513 -0.974788
C -2.398672 -3.180599 0.370515
C -1.049486 -3.236873 0.769317
C 4.608862 -0.953284 0.183568
C 5.389403 -0.912223 -0.997487
C 6.394341 0.061757 -1.118947
C 6.636567 1.000061 -0.100860
C 5.837161 0.952223 1.052239
C 4.825825 -0.010889 1.215740
C 0.649764 -3.047820 -2.696974
C -4.219224 -2.967570 -1.389598
C -0.733619 -3.519559 2.225434
C 5.148372 -1.906978 -2.117571
C 7.699369 2.066950 -0.269010
C 3.997012 -0.047416 2.481000
H 1.300777 -5.182711 0.799993
H 3.709216 -5.336912 1.451523
H 5.195316 -3.343609 1.150225
H -1.278089 5.171264 0.890758
H -3.681338 5.315233 1.564660
H -5.174953 3.334264 1.221904
H 6.999424 0.088084 -2.030025
H 6.010230 1.675453 1.854786

H 2.921641 0.071557 2.265172
H 4.098375 -1.017206 2.996269
H 4.306010 0.748795 3.176373
H 5.830978 -1.722380 -2.961182
H 5.292305 -2.944050 -1.771762
H 4.111453 -1.841464 -2.488271
H 8.044579 2.445484 0.706090
H 8.571683 1.680863 -0.820834
H 7.306418 2.927950 -0.839226
H -2.019982 -2.978256 -3.001202
H -3.176244 -3.243470 1.136049
H 0.222332 -3.458236 -3.625218
H 1.004264 -2.025600 -2.910262
H 1.530613 -3.646405 -2.419425
H -4.883395 -3.386359 -0.619201
H -4.514601 -1.915939 -1.533426
H -4.395268 -3.501302 -2.338281
H 0.238666 -3.110834 2.529854
H -1.509758 -3.094420 2.878126
H -0.702942 -4.610404 2.400553
H 1.987035 3.017799 -3.005422
H 3.208025 3.230749 1.114702
H -0.212437 3.182153 2.547564
H 1.535273 3.005543 2.883755
H 0.857355 4.591259 2.450021
H 4.885482 3.416835 -0.677977
H 4.510484 1.922216 -1.548677
H 4.369273 3.486580 -2.391087
H -0.267394 3.548348 -3.579766
H -1.009382 2.073309 -2.909606
H -1.564646 3.663603 -2.353710
H -6.949646 -0.031177 -2.091036
H -6.094173 -1.636122 1.818362
H -5.746832 1.778060 -2.976158
H -5.185405 2.975447 -1.772302
H -4.030577 1.841421 -2.483666
H -8.095314 -2.385788 0.611397
H -8.584149 -1.599024 -0.917133
H -7.334177 -2.861612 -0.924874
H -2.997337 -0.164776 2.309694
H -4.104598 1.036052 2.981908
H -4.445545 -0.704034 3.208069
H 0.145876 1.139569 2.888513

5-PH(TS)
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C -4.490752 -0.077962 0.105487
C -5.253311 -1.048356 0.823450
C -6.640143 -1.072288 0.569991
C -7.274457 -0.231251 -0.344252
C -6.474102 0.693427 -1.041572
N -3.132777 0.053614 0.345921
C -1.986106 0.296825 0.497417
Si -0.296518 0.975200 1.166835
P -1.105144 0.870162 3.203391
C -4.757480 -2.073715 1.879848

C -5.401291 -1.706752 3.246321
C -8.788115 -0.271206 -0.613772
C -9.399940 1.115864 -0.281711
C -4.308098 1.890066 -1.643968
C -3.701891 2.943915 -0.675733
C -0.267085 2.604600 0.109080
C -0.235348 2.514048 -1.314945
C -0.439758 3.653951 -2.110610
C -0.639129 4.922210 -1.546972
C -0.602862 5.024206 -0.148998
C -0.427175 3.902991 0.685312
C 0.097205 1.227622 -2.039807
C -0.391021 4.157030 2.181048
C -0.891029 6.136503 -2.416998
C 1.195714 -0.065747 0.553664
C 2.470625 0.590505 0.608064
C 3.591720 0.009003 -0.015373
C 3.518006 -1.220910 -0.690024
C 2.284201 -1.886398 -0.673789
C 1.135505 -1.365361 -0.043570
C 2.716000 1.849155 1.428660
Si 3.479673 1.301381 3.124420
C 5.384059 1.156184 3.091991
C 4.711440 -1.830549 -1.394502
Si 6.207298 -2.169622 -0.235413
C 7.407661 -0.691931 -0.116051
C -0.086831 -2.272100 -0.016051
Si 0.185264 -3.691967 1.287777
C 1.850554 -4.577236 1.008976
Si 3.593948 3.302676 0.506815
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C 3.156049 4.924658 1.406856
C 5.501721 3.176534 0.448109
Si 5.056755 -0.881156 -3.028408
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Si -0.695552 -2.964524 -1.712298
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C -5.215339 -3.499677 1.451305
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C -5.214570 2.690458 -2.616711
C -9.028425 -0.589741 -2.113539
C -9.516790 -1.338528 0.231620
C 2.960153 2.569593 4.450238
C 2.813684 -0.416394 3.586182
C 5.562804 -2.587297 1.505237
C 7.155316 -3.667570 -0.940110
C 0.183779 -2.963407 3.039164
C -1.190740 -5.022276 1.190569
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H -0.407711 3.550544 -3.199793
H 1.172281 1.005171 -1.956662

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H -0.163720 1.294706 -3.105927
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H 0.560065 3.827454 2.627760
H -1.969899 6.260302 -2.623075
H -0.543324 7.059024 -1.925583
H -0.379807 6.045103 -3.388872
H 4.549117 0.525690 0.044692
H 2.219347 -2.867883 -1.145272
H 1.751410 2.295327 1.733276
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H 4.414031 -2.841706 -1.739462
H -0.281369 -4.995993 -3.117190
H 1.252566 -4.402272 -2.448561
H 0.158501 -5.364729 -1.431321
H -0.552094 -2.359662 -4.124572
H -1.181953 -0.971641 -3.207717
H 0.561800 -1.332601 -3.189714
H -2.971400 -3.718266 -2.491223
H -2.806203 -3.988443 -0.738476
H -3.121519 -2.353182 -1.362015
H -0.965044 -5.806744 1.934854
H -2.186030 -4.619147 1.431353
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H 0.011183 -3.759342 3.785551
H 1.152174 -2.493767 3.266080
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H 3.071628 -1.903613 -4.219203
H 2.642410 -0.354728 -3.459962
H 8.002054 -3.942026 -0.287330
H 6.497673 -4.550695 -1.019030
H 7.559276 -3.461389 -1.944820
H 6.393485 -2.812813 2.196350
H 4.991238 -1.745732 1.925644
H 4.894409 -3.464750 1.484150
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H 7.884805 -0.477527 -1.086922
H 6.904620 0.229636 0.218538
H 3.678875 5.775147 0.935028
H 2.074335 5.124251 1.350344
H 3.444596 4.905927 2.470770
H 3.715408 3.990887 -1.903005
H 2.880248 2.426268 -1.753048
H 2.018920 3.925312 -1.354297
H 5.876092 3.962649 -0.231597

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H 5.870241 2.215121 0.057998
H 3.268810 -0.760896 4.531483
H 1.720954 -0.414111 3.710562
H 3.052919 -1.152017 2.802146
H 3.282248 2.243714 5.454675
H 3.396279 3.566098 4.267823
H 1.862515 2.680239 4.473121
H 5.710457 0.522788 3.935382
H 5.754772 0.686168 2.167799
H 5.885247 2.130977 3.196972
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H -7.240041 -1.783950 1.129130
H -10.481632 1.105034 -0.494313
H -9.254167 1.360893 0.782279
H -8.939471 1.913014 -0.885179
H -10.591728 -1.318910 -0.004905
H -9.136497 -2.349685 0.014986
H -9.399708 -1.144307 1.309808
H -10.111033 -0.601537 -2.321309
H -8.562143 0.164663 -2.765717
H -8.610637 -1.575480 -2.373016
H -4.583078 3.418117 -3.148225
H -5.689661 2.038635 -3.367423
H -5.997465 3.250763 -2.081351
H -3.147783 3.694667 -1.257576
H -4.515137 3.449112 -0.130246
H -3.001505 2.532976 0.055656
H -2.641101 1.990161 -3.042120
H -2.540232 0.579508 -1.981435
H -3.727580 0.591149 -3.302560
H -4.859165 -4.225152 2.200112
H -6.308420 -3.600382 1.381640
H -4.778501 -3.763392 0.475841
H -5.099480 -2.452914 3.999274
H -5.053003 -0.717331 3.581477
H -6.500811 -1.693227 3.194609
H -3.043482 -2.962776 2.827497
H -2.714306 -2.421701 1.174414
H -2.806491 -1.240687 2.521091
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6-PH(TS)
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C -0.567659 2.685463 0.433582
C -0.688218 2.712993 -0.991129
C -0.978411 3.920332 -1.651665
C -1.148884 5.126909 -0.954880
C -0.970161 5.107966 0.435848
Si -0.504745 0.984528 1.369888
P -1.417090 0.628065 3.338009
C -0.473430 1.481911 -1.855949
C -1.504308 6.406025 -1.684484
C -0.416982 4.021464 2.625897
C -2.151251 0.375042 0.584327
N -3.269764 0.183898 0.267942

C -4.576756 0.021367 -0.133078
C -5.025155 0.734251 -1.275648
C -6.349367 0.511855 -1.680307
C -7.206736 -0.356883 -0.986997
C -6.724271 -1.015575 0.162127
C -5.414357 -0.849409 0.621343
C -4.130194 1.709610 -2.032117
C -3.817405 1.187760 -3.452623
C -4.909842 -1.497717 1.906087
C -5.138387 -0.528514 3.093309
C -8.635295 -0.586278 -1.462625
C -9.659636 -0.144866 -0.391265
C 0.966870 -0.028251 0.678881
C 2.239450 0.606194 0.477160
C 3.267631 -0.089497 -0.195271
C 3.092877 -1.387875 -0.700319
C 1.870101 -2.019473 -0.433745
C 0.825589 -1.397992 0.276896
C 2.581275 2.000728 0.985873
Si 3.312303 3.203818 -0.339365
C 5.223783 3.142905 -0.394300
C 4.171700 -2.112475 -1.476194
Si 4.444972 -1.292522 -3.191139
C 2.717411 -1.024807 -3.953863
C -0.355560 -2.284311 0.643304
Si -1.236677 -3.137259 -0.838084
C -1.235182 -1.997608 -2.367448
Si 3.624290 1.926181 2.605988
C 2.616053 1.102174 3.989187
C 5.249592 0.960925 2.385392
C 4.017189 3.708954 3.172958
Si 5.688224 -2.527493 -0.372594
C 6.588906 -4.031364 -1.125991
C 6.919703 -1.079178 -0.240823
C 5.034028 -2.996545 1.355020
Si 0.204881 -3.437633 2.093038
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C 1.328061 -4.879888 1.546812
C 1.197411 -2.388105 3.322523
C -5.547890 -2.871963 2.188985
C -8.857247 -2.066785 -1.851814
C -4.758327 3.120738 -2.087181
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C 5.463268 -2.476353 -4.288070
C -0.462475 -4.804705 -1.360551
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H 5.409872 0.827944 -4.109315
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H 2.781062 -0.580579 -4.962146
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H 2.118314 -0.348461 -3.322190
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H 5.901022 -4.885627 -1.251075
H 7.016147 -3.800949 -2.115795
H 5.858270 -3.173195 2.067379
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H 2.638563 1.719358 -2.282665
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H 4.486892 3.693445 4.172029
H 4.703292 4.234778 2.489649
H 3.096288 4.311906 3.249461
H 5.788679 0.917060 3.348011
H 5.064249 -0.074258 2.061276
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H -8.708769 -2.722519 -0.978496
H -10.686606 -0.288637 -0.764459
H -9.542782 -0.743478 0.526645
H -9.525361 0.915860 -0.127569
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H -5.697783 3.118493 -2.663825
H -4.971096 3.495715 -1.074298
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H -3.322183 0.205238 -3.416906
H -4.741465 1.087731 -4.045499
H -4.761709 -0.983601 4.022243
H -4.600363 0.418982 2.944418
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H -5.044805 -3.331747 3.053487
H -6.617473 -2.775708 2.438473
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H -0.210444 0.882139 4.074069

7-PH(TS)
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O 1.032998 1.459779 0.489455
Si 1.114857 -0.014237 -0.329324
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O -0.440764 -0.695674 0.316296
P -1.908356 -0.200601 0.152679
N -2.249475 1.381700 -0.208910
C -2.089234 2.429796 0.823045
O 2.182304 -0.872510 0.637442
C 2.791975 -2.168766 0.408406
C 1.756100 -3.185329 -0.114035
N -2.586228 -1.070435 -1.105392
C -2.069843 -2.397187 -1.480539
N -2.591967 -0.426965 1.676714
C -2.007182 -1.393209 2.622555
C -3.951935 -0.816447 -1.579390
C 3.946333 -2.012822 -0.597639
C 3.322815 -2.611098 1.783196
C -4.050879 -0.298593 1.801529
C -2.009710 1.906164 -1.575323
H 2.144656 4.341798 -0.912143

H 1.358114 2.928097 -1.701047
H 0.460304 3.909592 -0.498225
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H 2.313449 2.606768 2.500220
H 4.081081 2.940102 0.030294
H 3.716523 1.340888 0.762260
H 3.422109 1.626967 -0.979867
H 2.218900 -4.181353 -0.208540
H 0.905863 -3.253890 0.583660
H 1.393538 -2.866517 -1.104204
H 3.833725 -3.584160 1.700243
H 4.036430 -1.866304 2.168737
H 2.491116 -2.704242 2.499969
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H -4.571411 -1.248816 1.572639
H -4.292302 -0.011469 2.838031
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H -3.963319 -0.872398 -2.681264
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H -4.284886 0.184384 -1.277112
H -2.782892 2.664499 -1.786741
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H -2.330196 2.026221 1.813383
H -1.053397 2.800057 0.824033
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8-PH(TS)
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C -2.079912 0.053756 -1.551171
C -3.430203 0.192651 -0.852014
Si -0.050267 -0.056691 0.672957
P -1.126223 0.559483 2.427894
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C 0.934735 2.407294 -0.339808
C 1.801831 2.728014 -1.567968
O 0.922518 -1.400059 0.758686
C 1.990674 -1.891946 -0.106109
C 3.219484 -0.977671 0.043928
C -0.380541 3.205651 -0.377864
C 1.709047 2.698549 0.958882
C 1.531137 -1.950881 -1.574796
C 2.302121 -3.305384 0.413314
H 4.070673 -1.391025 -0.521641

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H 3.121633 -3.753193 -0.171604
H 2.600152 -3.261876 1.471736
H 1.411328 -3.946973 0.325415
H 2.335327 -2.377311 -2.196246
H 0.639475 -2.589778 -1.669352
H 1.293081 -0.943825 -1.944625
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H -0.896366 3.056659 -1.341391
H -1.034463 2.882089 0.446840
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H 2.745060 2.160947 -1.531731
H 1.265782 2.460554 -2.492409
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H 2.618451 2.079340 1.004157
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H -2.151358 -0.465797 -2.519987
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H -3.338681 0.926427 -0.038731
H -4.301581 -1.828850 -0.943233
H -4.162349 -1.176887 0.712369
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H -1.955771 -2.081879 0.874157
H -2.355302 0.041261 1.883770

9-PH(TS)
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C 3.346063 2.114125 -0.571340
C 2.778149 2.559535 0.594578
Si -0.480817 0.461876 -0.844829
P -1.619353 2.208051 -1.426336
C 2.580456 0.665115 -2.503076
C 4.706293 2.371664 -1.137242
C 3.307679 3.485680 1.642998
C 0.549867 2.282419 1.726614
C -0.762206 -0.774545 0.633353
C 0.300970 -1.482137 1.287740
C 0.062110 -2.203098 2.472933
C -1.218235 -2.267389 3.034555
C -2.277761 -1.633687 2.379487
C -2.069674 -0.905153 1.189487
C 1.696580 -1.563343 0.735271
C 2.771730 -0.879396 1.356464
C 4.049077 -0.920567 0.770749
C 4.306438 -1.671038 -0.385747
C 3.259691 -2.445749 -0.914894
C 1.966637 -2.421661 -0.365257
C 2.603715 -0.148033 2.674279
C 0.936889 -3.414335 -0.871581
C 5.674511 -1.663875 -1.039471
C -3.304032 -0.359341 0.532372
C -3.928975 -1.119476 -0.486233

C -5.122097 -0.644287 -1.056455
C -5.719983 0.551674 -0.630055
C -5.107266 1.265599 0.412169
C -3.909759 0.831316 0.998611
C -3.356953 -2.451785 -0.935700
C -6.983045 1.070027 -1.288861
C -3.241069 1.683660 2.055531
Cl -0.320374 -0.854101 -2.541790
H 0.016392 3.214087 1.490163
H -0.174293 1.464975 1.805640
H 1.090907 2.385262 2.675529
H 4.312111 3.831693 1.363019
H 2.662605 4.372371 1.763270
H 3.380436 2.993132 2.627886
H 4.657952 2.860909 -2.124650
H 5.270583 3.029865 -0.462291
H 5.273237 1.432644 -1.251620
H 2.530614 -0.423683 -2.400333
H 1.785895 1.014961 -3.174961
H 3.560303 0.957544 -2.896324
H -3.294164 -1.704454 2.773757
H -1.390380 -2.827251 3.956836
H 0.895724 -2.732107 2.941278
H -5.599412 -1.230658 -1.847149
H -5.561556 2.196456 0.764102
H -4.025413 -2.933868 -1.665643
H -2.369607 -2.330642 -1.406299
H -3.225010 -3.134843 -0.079406
H -7.618124 1.611001 -0.568268
H -6.739519 1.773618 -2.104851
H -7.574158 0.248942 -1.725763
H -2.800699 1.076637 2.862452
H -2.428825 2.262234 1.580027
H -3.953129 2.397700 2.498626
H 3.454145 -3.097406 -1.772288
H 4.863644 -0.357335 1.236064
H 1.561618 0.135477 2.860774
H 2.912528 -0.797580 3.512566
H 3.237664 0.751160 2.709250
H 6.421759 -1.169909 -0.398215
H 6.025472 -2.688177 -1.248724
H 5.653943 -1.130699 -2.007239
H 1.090046 -3.632639 -1.938557
H 1.041514 -4.362481 -0.312893
H -0.090488 -3.060003 -0.734797
H -0.850611 3.041148 -0.531339

10-PH(TS)
C 3.744321 -0.584819 0.784279
C 3.136805 0.654222 0.432081
C 3.873057 1.599431 -0.331579
C 5.138781 1.220408 -0.821565
C 5.723144 -0.019527 -0.542263
C 5.020566 -0.897192 0.294483
C 1.794567 0.979206 1.038140
C 0.515314 0.648622 0.476325

C -0.636882 1.005502 1.257931
C -0.498500 1.646141 2.505492
C 0.755431 1.940541 3.040105
C 1.888703 1.594128 2.303992
Si 0.366593 -0.169424 -1.299997
P 1.831165 -1.318929 -2.400595
C -2.074499 0.751250 0.880027
C -2.782898 -0.375610 1.375718
C -4.124568 -0.551773 0.971838
C -4.820145 0.393093 0.213849
C -4.140077 1.567910 -0.144547
C -2.785177 1.763921 0.161397
C -2.313321 -1.418953 2.413902
C -3.138504 -1.224352 3.717290
C -6.299049 0.203400 -0.105767
C -6.636968 0.468377 -1.589386
C -2.142011 3.116813 -0.162408
C -2.370364 4.098901 1.014473
C 3.466933 3.058299 -0.595061
C 3.689417 3.940971 0.658754
C 7.074950 -0.405629 -1.127912
C 8.117643 -0.680958 -0.021060
C 3.061215 -1.579797 1.724772
C 3.603821 -1.417596 3.163804
C -1.197198 -1.381797 -1.152284
N -1.110714 -2.557190 -0.450434
C -2.270195 -3.311628 -0.587795
C -3.105262 -2.599713 -1.407178
N -2.426160 -1.431165 -1.755713
C 0.112975 -3.129470 0.114468
C -2.987744 -0.441046 -2.685869
C -4.499251 -2.914741 -1.849282
C -2.459641 -4.636744 0.080533
Cl -0.447077 1.385156 -2.565813
C -0.829797 -1.517464 2.824909
C -2.668247 3.771152 -1.459349
C -7.157784 1.114140 0.804871
C 2.063659 3.288853 -1.181404
C 6.935061 -1.629228 -2.063296
C 3.203119 -3.048172 1.263299
H 0.805955 -2.336452 0.384692
H -0.147154 -3.712642 1.006684
H 0.603068 -3.750523 -0.650481
H -3.452499 -5.039632 -0.161076
H -1.704191 -5.370887 -0.246085
H -2.384374 -4.548493 1.178185
H -5.208391 -2.147561 -1.498147
H -4.582866 -2.978778 -2.947058
H -4.808982 -3.882353 -1.431205
H -3.025322 0.539312 -2.206244
H -2.369589 -0.392295 -3.589972
H -4.003108 -0.755104 -2.946231
H 2.882940 1.802043 2.701034
H 0.848373 2.423464 4.015390
H -1.403243 1.882940 3.068133
H 5.693285 1.931072 -1.441729

H 5.471777 -1.855530 0.556339
H 4.175725 3.426848 -1.356258
H 7.435087 0.445813 -1.731183
H 1.990547 -1.338552 1.762714
H -4.681267 2.349321 -0.679098
H -4.655443 -1.447434 1.308179
H -2.600685 -2.398715 1.994109
H -6.560939 -0.845218 0.123770
H -1.060186 2.967586 -0.275723
H 1.952027 4.355189 -1.442455
H 1.918998 2.691293 -2.089951
H 1.268061 3.032829 -0.469392
H 3.600864 5.005261 0.381571
H 2.935544 3.729111 1.430133
H 4.690113 3.774476 1.089738
H 2.549489 -3.695639 1.871661
H 2.933404 -3.156311 0.201741
H 4.235568 -3.409425 1.393776
H 3.105729 -2.126932 3.846939
H 4.688210 -1.615759 3.185507
H 3.430469 -0.396145 3.534564
H 7.907373 -1.881079 -2.519440
H 6.583299 -2.506864 -1.496321
H 6.206386 -1.429840 -2.864207
H 9.094969 -0.932346 -0.465861
H 8.242705 0.197875 0.631499
H 7.801231 -1.530102 0.607021
H -1.924217 5.079238 0.777189
H -3.451098 4.241895 1.182937
H -1.918691 3.731069 1.945661
H -2.025872 4.626260 -1.720960
H -2.664661 3.067597 -2.302784
H -3.693202 4.156500 -1.324655
H -8.232145 0.956771 0.611711
H -6.954676 0.908790 1.867544
H -6.922645 2.173484 0.611179
H -7.713192 0.312784 -1.768809
H -6.394613 1.506334 -1.868056
H -6.074287 -0.200514 -2.259194
H -2.873843 -2.003687 4.451736
H -2.906320 -0.241860 4.159780
H -4.221898 -1.268774 3.532062
H -0.671821 -2.486666 3.327142
H -0.144432 -1.443128 1.980683
H -0.554906 -0.724040 3.532570
H 2.809802 -1.293588 -1.362629

11-PH(TS)
C 3.274877 0.590158 -1.213900
C 2.486325 -0.463360 -0.717689
C 3.009805 -1.518304 0.056849
C 4.376158 -1.475629 0.367053
C 5.202156 -0.427003 -0.076451
C 4.638550 0.583265 -0.872192
N 1.085134 -0.540019 -1.086246
C 0.000003 -0.120795 -0.365398

N -1.085102 -0.540058 -1.086262
C -0.682282 -1.204991 -2.235202
C 0.682355 -1.204967 -2.235191
C -2.486302 -0.463399 -0.717741
C -3.009782 -1.518320 0.056834
C -4.376128 -1.475636 0.367046
C -5.202128 -0.427017 -0.076488
C -4.638529 0.583210 -0.872277
C -3.274850 0.590101 -1.213984
C -2.126494 -2.635697 0.568340
C -2.696752 1.704492 -2.055766
C -6.666101 -0.379938 0.311637
Si -0.000029 1.154998 1.128806
P 0.000010 3.169153 0.391660
C 2.126532 -2.635706 0.568328
C 6.666155 -0.379960 0.311583
C 2.696767 1.704568 -2.055647
Cl 1.625343 0.510852 2.361357
Cl -1.625490 0.510919 2.361269
H -1.970456 1.329261 -2.794821
H -2.735831 -3.435736 1.013237
H 2.163816 2.424717 -1.410973
H 1.440133 -2.256601 1.343050
H -3.497349 2.236854 -2.590431
H -1.439988 -2.256531 1.342938
H 3.497357 2.236967 -2.590286
H 2.735892 -3.435819 1.013062
H -1.411214 -1.614403 -2.924151
H 1.411311 -1.614356 -2.924127
H -5.271486 1.394969 -1.239502
H -4.802278 -2.277118 0.975695
H 5.271505 1.395039 -1.239387
H 4.802314 -2.277130 0.975672
H -1.511122 -3.072874 -0.235433
H -2.163825 2.424677 -1.411109
H 1.970488 1.329344 -2.794724
H 1.511048 -3.072770 -0.235419
H 7.075966 -1.392370 0.453586
H 7.266765 0.137187 -0.453011
H 6.797993 0.166904 1.261641
H -7.076224 -1.392374 0.452569
H -6.797723 0.165918 1.262306
H -7.266578 0.138224 -0.452367
H 0.000030 2.650734 -0.951721

12-PH(TS)
C 3.025535 1.407795 -0.471517
C 2.486622 0.111035 -0.594204
C 3.258972 -1.065136 -0.580998
C 4.645977 -0.911700 -0.417749
C 5.220496 0.358019 -0.279821
C 4.416829 1.504244 -0.308905
N 1.069077 0.010329 -0.906348
C -0.004617 -0.047498 -0.059453
N -1.097373 0.041988 -0.884098
C -0.707022 0.146188 -2.208612

C 0.656728 0.124591 -2.222615
C -2.502284 0.171792 -0.538373
C -2.988498 1.470687 -0.265533
C -4.369605 1.596878 -0.047126
C -5.213768 0.479350 -0.096028
C -4.692263 -0.790527 -0.363438
C -3.316032 -0.975694 -0.593709
C -2.065255 2.687317 -0.222487
C -2.014536 3.380796 -1.605529
C -2.758889 -2.354832 -0.937375
C -3.030734 -2.681792 -2.425545
Si 0.152995 -0.463844 1.883000
P 1.947550 0.166246 2.837440
C 2.633090 -2.447046 -0.737111
C 3.141358 -3.435929 0.333466
C 2.162961 2.666946 -0.498239
C 2.390439 3.540628 0.755638
Cl -0.243539 -2.564693 1.729961
Cl -1.688032 0.383426 2.579410
C 2.884563 -2.993372 -2.162238
C 2.415582 3.474078 -1.792350
C -3.324896 -3.464574 -0.025918
C -2.448067 3.700824 0.875920
H 1.378091 0.194691 -3.026914
H -1.440954 0.236042 -2.999327
H 5.278104 -1.800075 -0.388292
H 6.300101 0.454545 -0.147596
H 4.869393 2.490164 -0.191857
H -5.356520 -1.654756 -0.392816
H -6.284138 0.600515 0.082845
H -4.785796 2.578991 0.178117
H 1.103533 2.372349 -0.497718
H 1.774619 4.370911 -1.814435
H 3.467051 3.799983 -1.844155
H 2.200983 2.869895 -2.689056
H 1.686479 4.389293 0.750393
H 2.240662 2.951465 1.672069
H 3.413623 3.949509 0.770532
H 1.546806 -2.355815 -0.595229
H 2.418365 -3.985460 -2.279063
H 2.466734 -2.320121 -2.929074
H 3.965955 -3.094529 -2.351125
H 2.594570 -4.387837 0.244750
H 4.215350 -3.647415 0.204999
H 2.978633 -3.029789 1.341896
H -1.670923 -2.338565 -0.783783
H -2.617727 -3.671934 -2.678447
H -4.115009 -2.696918 -2.623955
H -2.572060 -1.934743 -3.093608
H -2.811228 -4.413888 -0.244758
H -3.167260 -3.219424 1.033630
H -4.402243 -3.617608 -0.200418
H -1.050439 2.338022 0.015730
H -1.313432 4.231146 -1.577313
H -1.683151 2.687258 -2.394040
H -3.012115 3.762386 -1.878483

H -1.675667 4.484296 0.932256
H -3.407625 4.195214 0.653657
H -2.520393 3.206735 1.855021
H 2.251120 -1.197483 3.174885

13-PH(TS)
C 2.994510 1.396779 -0.029316
C 2.464466 0.116368 -0.293353
C 3.201394 -1.081041 -0.168567
C 4.543315 -0.956117 0.234451
C 5.106838 0.298112 0.503108
C 4.340560 1.461858 0.372196
N 1.085806 0.041959 -0.728428
C 0.005701 -0.000663 0.100600
N -1.076707 0.064406 -0.724001
C -0.680182 0.166010 -2.050398
C 0.686353 0.151009 -2.053349
C -2.453671 0.158559 -0.285900
C -3.224226 -1.022016 -0.219757
C -4.569343 -0.876688 0.165781
C -5.103145 0.380674 0.475764
C -4.301870 1.526433 0.410979
C -2.950593 1.440699 0.031764
C -2.648574 -2.382626 -0.606540
C -2.927355 -2.663790 -2.103688
C -2.094639 2.702769 -0.050366
C -2.534953 3.578004 -1.246748
Si -0.000215 -0.236917 2.031799
P -0.068749 -2.394774 2.312966
C 2.594523 -2.438154 -0.518437
C 3.094962 -3.580124 0.386907
C 2.177354 2.679261 -0.172110
C 2.098875 3.449664 1.164919
C 2.863795 -2.761424 -2.008867
C 2.752692 3.573080 -1.294814
C -2.127523 3.507909 1.267284
C -3.175322 -3.535037 0.271025
H 1.199371 0.611859 2.381624
H -1.407175 0.241867 -2.849003
H 1.411777 0.213108 -2.854742
H -4.721419 2.501749 0.662571
H -6.149431 0.465888 0.777075
H -5.200893 -1.762317 0.234360
H 4.782251 2.435995 0.588851
H 6.149336 0.366714 0.821268
H 5.149004 -1.854890 0.349264
H -1.560268 -2.348295 -0.451683
H -2.487667 -3.631818 -2.394390
H -4.013307 -2.706387 -2.290553
H -2.500349 -1.881851 -2.752481
H -2.660657 -4.465902 -0.014341
H -2.956808 -3.333575 1.329380
H -4.257702 -3.693765 0.131321
H -1.048685 2.411542 -0.221239
H -1.895795 4.473477 -1.319139
H -2.465235 3.020628 -2.194985

H -3.578844 3.908301 -1.121144
H -1.449708 4.373697 1.190828
H -3.140466 3.887499 1.477013
H -1.807188 2.878412 2.110680
H 1.148179 2.417716 -0.456966
H 2.142383 4.484586 -1.403679
H 3.785436 3.877198 -1.060055
H 2.765170 3.041401 -2.260131
H 1.468670 4.346180 1.043898
H 1.668147 2.813446 1.952271
H 3.099977 3.776485 1.489524
H 1.507668 -2.374947 -0.363705
H 2.403449 -3.727103 -2.274259
H 2.450537 -1.986962 -2.675452
H 3.948156 -2.830704 -2.197067
H 2.554953 -4.504215 0.128298
H 4.172535 -3.770265 0.248284
H 2.884888 -3.346519 1.440294
H -1.145735 0.684481 2.380014
H -0.077635 -2.255891 3.750121

14-PH(TS)
C 3.669628 1.388329 0.953024
C 3.917793 0.291383 0.092636
C 4.715986 0.377672 -1.068203
C 5.309203 1.623362 -1.345134
C 5.098923 2.725772 -0.508617
C 4.282340 2.610275 0.623450
N 3.351693 -0.988588 0.459082
C 2.023743 -1.308039 0.315281
N 1.871143 -2.472582 1.029668
C 3.081110 -2.867908 1.594005
C 4.008441 -1.931843 1.239586
Si 0.754664 -0.357246 -0.810418
P 1.244465 -0.729133 -2.910875
C 0.606799 -3.108431 1.322754
C 0.044109 -2.897093 2.600967
C -1.176368 -3.538884 2.880420
C -1.814347 -4.322990 1.914304
C -1.234328 -4.500917 0.651523
C -0.003353 -3.905852 0.327649
C 0.716379 -2.030645 3.666507
C -0.261260 -1.035643 4.330122
C 0.671855 -4.132551 -1.023312
C -0.305490 -4.550385 -2.138447
C 4.949247 -0.834363 -1.966446
C 6.231736 -1.587762 -1.537990
C 2.828265 1.255018 2.221818
C 3.737651 0.958518 3.437602
Si -0.782700 0.222898 0.660789
C -1.957687 1.209828 -0.525961
N -1.992475 2.571854 -0.709513
C -3.172601 2.965167 -1.335735
C -3.892322 1.830693 -1.566962
N -3.136628 0.766984 -1.081729
C -1.075089 3.509374 -0.104107

C -1.412997 4.018659 1.168734
C -0.575003 5.007501 1.715141
C 0.555604 5.451221 1.021818
C 0.884439 4.896077 -0.222262
C 0.078127 3.908694 -0.817102
C -2.619226 3.519611 1.960752
C -3.658453 4.644493 2.163591
C 0.422216 3.292285 -2.169988
C 1.931349 3.318418 -2.478521
C -3.574524 -0.610014 -1.081013
C -3.423006 -1.370588 -2.262957
C -3.880102 -2.701599 -2.228449
C -4.449499 -3.242932 -1.070204
C -4.580954 -2.462014 0.083769
C -4.144782 -1.126040 0.106366
C -2.830965 -0.773996 -3.539231
C -3.954003 -0.168364 -4.418834
C -4.341627 -0.262007 1.351515
C -4.103606 -1.034135 2.665337
C -2.024957 -1.787790 -4.375016
C -5.745673 0.386865 1.331954
C 1.386279 -2.921017 4.739609
C 1.803821 -5.180280 -0.887879
C 5.026264 -0.465113 -3.461423
C 1.932654 2.480853 2.484471
C -0.368522 3.983491 -3.306583
C -2.175980 2.915492 3.312478
H -4.860107 1.673770 -2.024924
H -3.378565 4.007670 -1.545123
H 1.787968 5.224323 -0.735180
H 1.197274 6.218770 1.460572
H -0.813045 5.419199 2.697721
H 0.118717 2.233510 -2.141982
H -0.132628 3.500705 -4.268793
H -1.455164 3.913487 -3.146093
H -0.094349 5.050074 -3.374234
H 2.121324 2.738440 -3.393721
H 2.292074 4.347380 -2.650667
H 2.514252 2.872299 -1.660876
H -3.107243 2.715383 1.393505
H -3.051357 2.509642 3.846748
H -1.454798 2.101184 3.143923
H -1.707665 3.680857 3.953072
H -4.529364 4.260399 2.719856
H -3.224749 5.479361 2.737913
H -4.008237 5.040391 1.196429
H -5.020402 -2.894578 0.982938
H -4.790299 -4.280989 -1.066466
H -3.777177 -3.321586 -3.118810
H -2.130690 0.023743 -3.248017
H -3.517641 0.278656 -5.327103
H -4.660002 -0.957742 -4.727398
H -4.525609 0.611655 -3.894364
H -1.546006 -1.258066 -5.212049
H -1.225862 -2.242398 -3.777183
H -2.675122 -2.573162 -4.797745

H -3.599901 0.547119 1.332685
H -4.114292 -0.327141 3.510495
H -4.892860 -1.782791 2.846322
H -3.129102 -1.543215 2.642332
H -5.879330 1.032819 2.216087
H -5.885233 1.002073 0.428550
H -6.529896 -0.388209 1.345847
H 3.156063 -3.769921 2.188124
H 5.062084 -1.837854 1.470124
H -1.751926 -5.100655 -0.096047
H -2.773273 -4.793543 2.142045
H -1.638482 -3.398762 3.858787
H 1.135269 -3.186382 -1.341966
H 0.215526 -4.515305 -3.106948
H -0.672737 -5.579850 -1.985062
H -1.171143 -3.874401 -2.184549
H 2.308365 -5.311367 -1.858929
H 2.557184 -4.867393 -0.148996
H 1.390307 -6.153664 -0.574080
H 1.502698 -1.432431 3.185391
H 0.292525 -0.397505 5.038908
H -0.735029 -0.397733 3.569107
H -1.048373 -1.559913 4.896388
H 1.897595 -2.294915 5.489538
H 0.628094 -3.531351 5.257522
H 2.125754 -3.605024 4.293916
H 4.111943 3.479020 1.259992
H 5.563827 3.685144 -0.747334
H 5.929871 1.731325 -2.234846
H 2.144799 0.405544 2.094841
H 1.282484 2.275752 3.349456
H 2.524614 3.382023 2.714459
H 1.293653 2.685688 1.615285
H 3.123328 0.820546 4.343323
H 4.331504 0.044118 3.279439
H 4.433545 1.795493 3.615115
H 4.079109 -1.499444 -1.855428
H 6.383393 -2.469979 -2.181544
H 7.113986 -0.932804 -1.635976
H 6.176623 -1.931083 -0.493114
H 5.081322 -1.388724 -4.058605
H 4.124906 0.086313 -3.763413
H 5.922257 0.136906 -3.689437
H 1.709374 0.604191 -3.195247

15-PH(TS)
C -4.708336 1.563728 0.892199
C -4.439610 0.656649 -0.155705
C -4.864329 0.863132 -1.489856
C -5.497659 2.084294 -1.780186
C -5.717198 3.039576 -0.782015
C -5.344647 2.768975 0.537136
N -3.777805 -0.596431 0.157910
C -2.435216 -0.903805 0.108777
N -2.378263 -2.205014 0.538505
C -3.645180 -2.697293 0.821194

C -4.521404 -1.683268 0.586103
Si -0.971986 0.223142 -0.677266
P -1.145348 0.147893 -2.841477
C -1.234088 -3.085297 0.688846
C -0.969754 -3.988409 -0.360568
C 0.030482 -4.951223 -0.139513
C 0.739768 -4.986888 1.064163
C 0.456576 -4.068168 2.082416
C -0.548811 -3.098829 1.926731
C -1.734538 -3.961282 -1.681496
C -2.710634 -5.158642 -1.760307
C -0.951496 -2.178688 3.078535
C -2.062524 -2.846854 3.925929
C -4.766759 -0.233434 -2.549602
C -4.569248 0.306973 -3.978987
C -4.495985 1.334699 2.396662
C -5.805376 0.759837 2.998983
Si 1.073776 -0.356825 0.518858
Cl 1.643448 -1.997029 -0.820692
C 2.505499 0.918521 0.049852
N 2.591950 2.281616 0.335592
C 3.907118 2.729772 0.210301
C 4.671098 1.661579 -0.124275
N 3.830350 0.558996 -0.215266
C 1.567549 3.302768 0.554693
C 1.004568 3.923832 -0.591085
C 0.187337 5.050870 -0.404012
C -0.092898 5.537269 0.872788
C 0.453074 4.896288 1.986649
C 1.307476 3.781334 1.866632
C 1.247699 3.409504 -2.006514
C 2.488951 4.096256 -2.625704
C 1.836533 3.201092 3.184892
C 3.373897 3.220321 3.338702
C 4.434866 -0.726817 -0.547887
C 4.686818 -1.016377 -1.916401
C 5.337028 -2.224622 -2.225242
C 5.753867 -3.111633 -1.231158
C 5.529099 -2.782886 0.103476
C 4.872463 -1.594076 0.486269
C 4.383156 -0.120087 -3.124665
C 5.602402 0.788435 -3.425916
C 4.699554 -1.456503 2.008723
C 3.595037 -2.430215 2.493511
C 3.099412 0.721690 -3.091383
C 4.469554 -0.060235 2.605415
C 1.239224 1.813549 3.493308
C 0.036192 3.591833 -2.947259
Cl -1.539858 2.119771 0.205621
C -0.785695 -3.938777 -2.899862
C 0.219454 -1.766925 3.991293
C -6.035129 -1.122801 -2.497662
C -3.299085 0.492310 2.882570
H 4.154458 3.767766 0.389115
H 5.735021 1.560725 -0.294972
H 5.518099 -2.461932 -3.276164

H 6.257666 -4.043932 -1.495244
H 5.863480 -3.461039 0.892478
H 4.285938 -0.813304 -3.976871
H 2.885745 1.086276 -4.109150
H 2.227088 0.152718 -2.742138
H 3.244112 1.600030 -2.455665
H 5.440677 1.329871 -4.372969
H 5.729716 1.537219 -2.627787
H 6.531714 0.202312 -3.508321
H 5.652744 -1.821050 2.431976
H 4.526620 -0.130451 3.703675
H 5.224910 0.665605 2.269653
H 3.475214 0.320767 2.350565
H 3.526653 -2.400445 3.594211
H 2.621873 -2.143929 2.071911
H 3.813460 -3.462033 2.178332
H 0.225285 5.271514 2.986954
H -0.740157 6.407496 1.002190
H -0.254734 5.531612 -1.275869
H 1.429510 2.331316 -1.939222
H 2.663050 3.712664 -3.643347
H 2.321243 5.184707 -2.686638
H 3.398055 3.917316 -2.032528
H 0.211230 3.013311 -3.866101
H -0.890018 3.223158 -2.485967
H -0.099475 4.649893 -3.230088
H 1.458236 3.878901 3.968737
H 3.634161 2.968547 4.380053
H 3.867554 2.492836 2.686749
H 3.776514 4.222523 3.116907
H 1.570867 1.471426 4.488339
H 0.139027 1.856355 3.482409
H 1.542859 1.059710 2.754672
H -5.595999 -1.613852 0.690335
H -3.782475 -3.717059 1.156169
H -5.819790 2.286951 -2.801121
H -6.195138 3.989685 -1.030582
H -5.546683 3.501038 1.322712
H -3.888432 -0.851719 -2.321063
H -4.378005 -0.538357 -4.658785
H -5.470148 0.829780 -4.342736
H -3.701948 0.980950 -4.012226
H -5.960665 -1.924131 -3.251418
H -6.173352 -1.591839 -1.511424
H -6.933273 -0.522618 -2.719212
H -4.360240 2.342070 2.824663
H -5.725237 0.703027 4.097469
H -6.674040 1.384382 2.738904
H -5.986274 -0.259126 2.619087
H -3.206148 0.621905 3.973532
H -3.451626 -0.579732 2.699876
H -2.358233 0.807244 2.415491
H 1.023560 -4.103418 3.012260
H 1.526668 -5.730051 1.209837
H 0.267491 -5.660836 -0.933156
H -1.358007 -1.257233 2.644065

H -0.140165 -1.029031 4.726130
H 0.620231 -2.627812 4.551416
H 1.024866 -1.311422 3.400233
H -2.375524 -2.171362 4.738974
H -2.950075 -3.089137 3.322513
H -1.686039 -3.780747 4.375306
H -2.330590 -3.037987 -1.726082
H -3.271486 -5.129082 -2.708857
H -2.157739 -6.111347 -1.714962
H -3.433934 -5.144009 -0.928340
H -1.382272 -3.878243 -3.824526
H -0.117944 -3.067490 -2.852208
H -0.176583 -4.856159 -2.947154
H -1.713551 -1.175623 -2.783059

16-PH(TS)
C -3.028146 1.997015 0.032230
C -3.215997 0.629852 -0.310218
C -3.993793 0.271999 -1.453197
C -4.628448 1.295889 -2.177165
C -4.513272 2.637218 -1.808019
C -3.704623 2.974195 -0.723351
N -2.714664 -0.430214 0.554133
C -1.428287 -0.857542 0.689725
C -1.512106 -2.243619 1.395986
C -2.741895 -2.063496 2.313375
C -3.644123 -1.012646 1.615071
Si 0.077519 -0.120008 -0.130223
P -0.154343 0.416227 -2.231644
C -4.021479 0.122484 2.586477
C -4.938537 -1.614017 1.052769
C -1.840285 -3.270202 0.265647
C -0.267464 -2.794881 2.138534
C -4.127576 -1.146930 -2.009003
C -3.353198 -1.288713 -3.341299
C -2.071698 2.504464 1.112154
C -0.969252 3.367178 0.441425
C 1.479554 -0.047669 1.052806
N 2.811988 0.028366 0.654188
C 3.799055 0.002327 1.795740
C 2.862172 -0.113608 3.019173
C 1.478518 0.387498 2.544062
C 3.258133 -0.136344 -0.709527
C 3.660530 1.002590 -1.459855
C 4.145718 0.808145 -2.765563
C 4.218281 -0.465438 -3.334529
C 3.787783 -1.572076 -2.597576
C 3.302877 -1.437194 -1.284499
C 3.514381 2.439155 -0.960132
C 2.433898 3.194839 -1.768878
C 2.805909 -2.698539 -0.579048
C 1.601063 -3.308099 -1.335768
C 1.412316 1.946230 2.571177
C 0.360727 -0.093300 3.489620
C 4.728950 -1.222403 1.689329
C 4.688464 1.259436 1.856089

C -5.595586 -1.580397 -2.242012
C -2.778106 3.344749 2.201551
C 3.913005 -3.772718 -0.453643
C 4.840135 3.233918 -1.026145
H 2.772597 -1.171535 3.315898
H 3.241774 0.453480 3.883057
H 3.818644 -2.566495 -3.047261
H 4.591742 -0.594008 -4.352929
H 4.445046 1.679634 -3.350235
H 2.460740 -2.422780 0.425701
H 3.532448 -4.639419 0.112681
H 4.215573 -4.131164 -1.450584
H 4.809000 -3.387906 0.053195
H 1.187578 -4.153754 -0.761371
H 0.811768 -2.559486 -1.497570
H 1.916053 -3.687124 -2.321892
H 3.180516 2.400974 0.082015
H 2.271348 4.194189 -1.329318
H 2.762822 3.329462 -2.812821
H 1.486115 2.635318 -1.786182
H 4.701000 4.227778 -0.569674
H 5.670290 2.727707 -0.511337
H 5.141898 3.389227 -2.074529
H -0.617131 -0.093508 2.984298
H 0.560467 -1.093926 3.885785
H 0.294501 0.593907 4.349328
H 0.368266 2.265617 2.470572
H 1.794708 2.314177 3.539811
H 1.984753 2.409522 1.759301
H 5.287618 -1.211894 0.742047
H 5.449374 -1.198784 2.522376
H 4.154242 -2.154678 1.752911
H 5.286899 1.340000 0.940467
H 4.106225 2.179537 1.985788
H 5.377577 1.163408 2.710608
H -2.412720 -1.684808 3.293503
H -3.277660 -3.010967 2.478477
H -3.573423 4.023462 -0.454649
H -5.026731 3.414837 -2.377580
H -5.213161 1.026003 -3.057473
H -1.588310 1.641067 1.590996
H -0.284067 3.777254 1.198393
H -0.388824 2.778924 -0.283776
H -1.423391 4.216694 -0.091689
H -2.043907 3.652024 2.964762
H -3.210674 4.260292 1.766923
H -3.586017 2.789853 2.698496
H -3.670194 -1.835522 -1.295322
H -3.432899 -2.328186 -3.703826
H -3.788102 -0.623823 -4.106062
H -2.295059 -1.022491 -3.205742
H -5.618781 -2.640693 -2.542572
H -6.230640 -1.456724 -1.353580
H -6.044980 -0.997853 -3.061940
H -4.606758 0.898603 2.073348
H -4.627422 -0.296309 3.405743

H -3.118698 0.581369 3.012950
H -5.502192 -0.851354 0.500963
H -4.753495 -2.472646 0.396610
H -5.554631 -1.954141 1.899847
H 0.642286 -2.243923 1.861506
H -0.398313 -2.743489 3.227314
H -0.104890 -3.852866 1.881025
H -1.005212 -3.338210 -0.443114
H -1.995878 -4.257761 0.731932
H -2.745335 -3.003610 -0.288642
H 0.858669 -0.508955 -2.668505

17-PH(TS)
C -3.454690 0.270594 2.188579
C -3.404325 -0.122529 0.824277
C -4.004699 -1.338068 0.393625
C -4.677876 -2.123431 1.346190
C -4.764365 -1.733595 2.685891
C -4.150077 -0.548988 3.096785
N -2.775786 0.745954 -0.148654
C -1.422867 0.786217 -0.421297
C -1.199387 1.965999 -1.406758
C -2.623435 2.263141 -1.940027
C -3.601183 1.796802 -0.849258
C -0.604673 3.176519 -0.622380
C -0.352169 4.417093 -1.500842
C 0.584200 4.068200 -2.672248
C 0.022897 2.882900 -3.478526
C -0.245549 1.652579 -2.584261
Si -0.095291 0.000603 0.628835
P -0.470488 -1.832208 1.829881
C -4.883459 1.210637 -1.462772
C -4.037217 2.939019 0.093823
C -3.926570 -1.874409 -1.038408
C -5.331374 -2.093575 -1.655037
C -2.785339 1.530167 2.739537
C -3.824251 2.522576 3.351606
C 1.312341 -0.723844 -0.457752
N 2.643165 -0.423725 -0.303781
C 3.536580 -1.027590 -1.378165
C 2.496128 -1.610841 -2.350416
C 1.213094 -1.856098 -1.521643
C 1.234356 -3.275420 -0.847281
C 1.222749 -4.432811 -1.865276
C -0.029556 -4.343444 -2.756419
C -0.125600 -2.960164 -3.426559
C -0.043066 -1.791465 -2.416836
C 3.339415 0.246958 0.790304
C 3.816604 1.581467 0.641935
C 4.808055 2.048890 1.525471
C 5.300087 1.255817 2.562810
C 4.741126 -0.005945 2.768892
C 3.759696 -0.533280 1.908344
C 3.209408 2.610538 -0.309907
C 4.234890 3.325795 -1.222128
C 3.144155 -1.873020 2.303295

C 4.177427 -3.010083 2.482391
C 4.358786 0.069384 -2.071923
C 4.514908 -2.082210 -0.830314
C 2.386343 -1.682324 3.643020
C 2.510001 3.690958 0.557622
C -3.173275 -3.225082 -1.102122
C -1.726574 1.187095 3.816734
H 2.276271 -0.873017 -3.139901
H 2.876762 -2.515776 -2.840635
H 5.182194 3.066520 1.402233
H 6.082203 1.632409 3.225777
H 5.066212 -0.609723 3.617367
H 2.453803 2.110128 -0.934063
H 3.709490 4.026642 -1.891008
H 4.938799 3.917214 -0.615052
H 4.819616 2.631607 -1.838277
H 1.978561 4.411712 -0.080737
H 1.798820 3.236909 1.262577
H 3.263844 4.242608 1.140612
H 2.404655 -2.170094 1.551333
H 1.833131 -2.599425 3.892871
H 3.100528 -1.460991 4.454365
H 1.662379 -0.858012 3.579534
H 3.646859 -3.946456 2.719607
H 4.790347 -3.173225 1.585815
H 4.857579 -2.791881 3.321966
H -2.795473 1.677178 -2.858203
H -2.777460 3.321500 -2.188709
H -5.132881 -3.062761 1.026473
H -5.294295 -2.359196 3.407648
H -4.189504 -0.250603 4.146133
H -3.367487 -1.151454 -1.649045
H -3.134260 -3.579977 -2.145408
H -2.147495 -3.141435 -0.724595
H -3.694536 -3.986448 -0.500401
H -5.235526 -2.367722 -2.718935
H -5.843102 -2.923670 -1.141585
H -5.971654 -1.205461 -1.576728
H -2.252617 2.022614 1.917084
H -1.242155 2.116640 4.161048
H -2.205787 0.709849 4.687283
H -0.963661 0.504099 3.422019
H -3.541747 3.565704 3.137075
H -4.840191 2.358152 2.962853
H -3.870898 2.407630 4.447059
H 0.704721 1.258732 -2.187393
H -0.702102 0.866122 -3.200291
H 0.718734 2.602486 -4.287130
H -0.922525 3.187964 -3.961543
H 1.570727 3.788224 -2.267908
H 0.734343 4.943486 -3.326375
H 0.085540 5.217309 -0.881216
H -1.303586 4.813226 -1.895881
H 0.343968 2.828893 -0.204618
H -1.240250 3.429290 0.236763
H -0.936948 -1.766902 -1.778485

H -0.022507 -0.857069 -2.984015
H -1.068125 -2.875971 -3.993614
H 0.694975 -2.857230 -4.159979
H -0.921115 -4.504405 -2.128357
H -0.020758 -5.137080 -3.522814
H 1.231812 -5.387676 -1.313496
H 2.130829 -4.426000 -2.493864
H 0.336809 -3.342662 -0.221037
H 2.085471 -3.361839 -0.162109
H 5.093270 0.514609 -1.387326
H 4.897838 -0.386019 -2.918086
H 3.700354 0.857206 -2.461659
H 5.171640 -1.639303 -0.068835
H 3.996009 -2.940761 -0.393617
H 5.140062 -2.443207 -1.662238
H -4.566286 3.702015 -0.499394
H -4.727884 2.555762 0.855065
H -3.194995 3.419574 0.601755
H -5.451864 2.026980 -1.935570
H -4.653214 0.461028 -2.228865
H -5.513754 0.752903 -0.687082
H -1.502805 -2.399160 1.013427

18-PH(TS)

C	-3.224932	0.218252	-1.358397
C	-2.946352	-0.186418	-0.029054
C	-3.619881	0.346863	1.093114
C	-4.622123	1.305097	0.851972
C	-4.919079	1.726140	-0.447161
C	-4.222227	1.191741	-1.539824
N	-1.954869	-1.204742	0.189782
C	-0.580617	-1.016769	0.090476
N	-0.029330	-2.229651	0.492905
C	-1.039767	-3.138722	0.813580
C	-2.228656	-2.505497	0.625453
N	0.078829	0.000550	-0.359199
Si	0.615108	1.529979	0.090764
P	0.017296	2.702467	1.801247
C	1.380952	-2.497403	0.473241
C	1.908536	-3.241348	-0.607523
C	3.294056	-3.485270	-0.611446
C	4.111977	-2.994684	0.413084
C	3.562720	-2.243373	1.460013
C	2.183162	-1.973414	1.513742
C	1.020702	-3.678706	-1.773747
C	1.493737	-4.974988	-2.462843
C	1.564798	-1.159497	2.651260
C	2.571257	-0.237302	3.365620
C	-3.323863	-0.108302	2.521098
C	-3.167505	1.073584	3.501760
C	-2.487067	-0.410662	-2.541873
C	-3.000227	-1.846010	-2.814548
C	1.337011	2.318507	-1.662868
C	1.369362	3.735976	-1.364337
C	2.422786	3.998390	-0.474480
C	3.105429	2.784970	-0.201068

C	2.487807	1.716169	-0.918922
C	0.913629	-2.525358	-2.801853
C	0.871792	-2.088601	3.676901
C	-4.431621	-1.070294	3.014585
C	-2.567885	0.421467	-3.836591
C	0.314461	4.726382	-1.768636
C	2.651410	5.298894	0.244271
C	4.191804	2.632861	0.824904
C	3.137032	0.395519	-1.278323
C	0.782092	1.725969	-2.946462
H	-0.804820	-4.144484	1.139750
H	-3.248157	-2.841463	0.762316
H	4.216445	-1.856395	2.241578
H	5.186160	-3.191682	0.391825
H	3.737329	-4.055396	-1.428234
H	0.007118	-3.866091	-1.388509
H	0.745208	-5.289195	-3.207287
H	2.446209	-4.823509	-2.996188
H	1.631156	-5.791886	-1.736491
H	0.215774	-2.799011	-3.610719
H	0.558805	-1.603071	-2.320808
H	1.901740	-2.321596	-3.246466
H	0.791995	-0.503971	2.221894
H	2.025730	0.424697	4.054394
H	3.302728	-0.815431	3.955161
H	3.117774	0.391450	2.646256
H	0.404983	-1.483578	4.471216
H	0.088346	-2.697955	3.202153
H	1.608189	-2.765491	4.141763
H	-4.461227	1.536330	-2.545779
H	-5.692226	2.479696	-0.612796
H	-5.158929	1.735125	1.698445
H	-2.369051	-0.653997	2.517737
H	-4.203401	-1.420909	4.034646
H	-5.404165	-0.551467	3.037863
H	-4.534724	-1.950008	2.359424
H	-2.887308	0.685477	4.495251
H	-2.381574	1.759173	3.151117
H	-4.113216	1.628822	3.616181
H	-1.424676	-0.475107	-2.269930
H	-1.899517	-0.016074	-4.594419
H	-3.589849	0.424082	-4.250837
H	-2.261784	1.464286	-3.663498
H	-2.430967	-2.296534	-3.644844
H	-2.888836	-2.492662	-1.931986
H	-4.065542	-1.823014	-3.098559
H	1.054802	2.095013	2.599848
H	0.566434	0.655754	-2.825757
H	-0.152416	2.227797	-3.237827
H	1.507978	1.844990	-3.770389
H	0.770559	5.678357	-2.088350
H	-0.308572	4.347316	-2.592943
H	-0.346950	4.955186	-0.913278
H	3.712378	5.436425	0.508900
H	2.331266	6.158173	-0.366252
H	2.060602	5.307810	1.178525

H	4.954561	3.421890	0.715794
H	3.770168	2.729990	1.842233
H	4.690182	1.654665	0.751545
H	3.814513	0.053519	-0.482302
H	2.384186	-0.388930	-1.425978
H	3.722961	0.498086	-2.209934

19-PH(TS)

C	-2.912489	-0.462403	1.191703
C	-2.617508	-1.148358	-0.025807
C	-3.629636	-1.275484	-1.020168
C	-4.868847	-0.642466	-0.818232
C	-5.137990	0.120345	0.323549
C	-4.151913	0.184313	1.321881
C	-1.282331	-1.806522	-0.206904
C	-0.035152	-1.103569	-0.206200
C	1.168750	-1.881368	-0.248799
C	1.111258	-3.278055	-0.395480
C	-0.113723	-3.951350	-0.434699
C	-1.292168	-3.215200	-0.305607
Si	0.214525	0.793366	0.045894
P	0.902242	1.639064	1.901312
C	2.519187	-1.271206	0.027653
C	3.377124	-0.824875	-1.014668
C	4.590866	-0.201422	-0.675409
C	4.997125	-0.052577	0.659545
C	4.186258	-0.594607	1.665782
C	2.954146	-1.206333	1.383685
C	3.065087	-1.130261	-2.481035
C	3.545589	-2.561250	-2.834546
C	6.285439	0.683342	1.005273
C	6.182590	2.173985	0.605176
C	2.158339	-1.869463	2.513361
C	2.608573	-3.345539	2.663918
C	-3.441899	-2.070695	-2.319644
C	-4.292741	-3.363924	-2.273185
C	-6.457102	0.866468	0.479999
C	-7.226391	0.412841	1.741553
C	-1.991700	-0.575687	2.412456
C	-2.213809	-1.956708	3.077436
C	-1.074150	2.056325	-1.143247
C	-0.972190	3.306164	-0.455650
C	0.331901	3.836209	-0.622816
C	1.077931	2.949176	-1.423409
C	0.252327	1.803970	-1.763856
C	-2.009494	3.875410	0.460392
C	-2.359406	1.523163	-1.723098
C	0.372029	1.001651	-3.046815
C	2.536944	3.060203	-1.756483
C	0.838437	5.063018	0.084143
C	3.709061	-0.147051	-3.483808
C	2.279268	-1.172392	3.884294
C	7.519132	0.026362	0.345817
C	-3.808977	-1.275415	-3.596374
C	-6.217586	2.394363	0.509394
C	-2.158839	0.549061	3.451451

H	2.044975	-3.840025	-0.424510
H	-0.147168	-5.039488	-0.521021
H	-2.252932	-3.728931	-0.267340
H	-5.640790	-0.723801	-1.587330
H	-4.370734	0.731464	2.238684
H	4.517175	-0.510651	2.702324
H	5.243723	0.166984	-1.467604
H	1.095127	-1.859574	2.233423
H	1.588226	-1.657214	4.593703
H	3.296499	-1.270807	4.299814
H	2.014851	-0.108753	3.806022
H	2.025073	-3.838497	3.459745
H	2.473218	-3.913750	1.733448
H	3.675107	-3.387420	2.941627
H	6.417145	0.633451	2.099881
H	7.096219	2.718395	0.897160
H	6.059893	2.270265	-0.486506
H	5.315734	2.650713	1.089441
H	8.440600	0.555795	0.639964
H	7.609897	-1.030499	0.642792
H	7.440150	0.066925	-0.752958
H	1.973865	-1.105806	-2.612130
H	3.356252	-2.773082	-3.900684
H	4.629013	-2.648201	-2.650112
H	3.029323	-3.321955	-2.235050
H	3.278016	-0.301685	-4.485649
H	3.559936	0.901461	-3.191026
H	4.794598	-0.322190	-3.560755
H	-0.942353	-0.549438	2.094393
H	-1.351611	0.473727	4.194393
H	-2.091803	1.542457	2.982722
H	-3.123183	0.470774	3.981867
H	-1.537789	-2.068819	3.941522
H	-3.254497	-2.049612	3.431331
H	-2.011094	-2.773304	2.367891
H	-2.386407	-2.362154	-2.409656
H	-3.649558	-1.912522	-4.481864
H	-4.867905	-0.972142	-3.589614
H	-3.196043	-0.369948	-3.710352
H	-4.126212	-3.965562	-3.182239
H	-4.048723	-3.981090	-1.395257
H	-5.364400	-3.111508	-2.217661
H	-7.080634	0.635692	-0.401248
H	-7.174624	2.936463	0.588161
H	-5.595441	2.668497	1.377086
H	-5.698148	2.728843	-0.403076
H	-8.192912	0.938657	1.812332
H	-7.416139	-0.671892	1.719182
H	-6.647744	0.639943	2.651633
H	2.251880	1.711499	1.405484
H	0.083619	5.866678	0.071490
H	1.051751	4.817111	1.138593
H	1.761015	5.452188	-0.371765
H	-2.134973	4.959548	0.301081
H	-2.982737	3.378395	0.338645
H	-1.671852	3.737191	1.505531

H	-2.675566	2.159269	-2.570084
H	-2.216315	0.509114	-2.101513
H	-3.169307	1.493624	-0.984530
H	3.122795	2.309808	-1.197134
H	2.712125	2.878884	-2.830169
H	2.933470	4.054017	-1.504425
H	1.413463	0.938627	-3.377839
H	-0.013484	-0.021683	-2.923646
H	-0.216567	1.489306	-3.843949

20-PH(TS)

C	-2.703969	-1.100278	-0.022875
C	-1.838951	-0.675264	1.045653
C	-1.760343	0.815186	0.947985
C	-2.590452	1.181110	-0.174335
C	-3.157254	0.024807	-0.745568
Si	-0.126538	-0.074586	-0.046440
P	-0.027875	-0.158393	-2.201512
C	1.496528	-0.049608	1.079408
C	2.237352	-1.188394	0.438607
C	3.119870	-0.673823	-0.481631
C	3.041019	0.780691	-0.465793
C	2.110803	1.181415	0.468000
C	-1.530819	1.751869	2.124060
C	-2.686277	2.558331	-0.760500
C	-3.927863	-0.014388	-2.033989
C	-2.937334	-2.528260	-0.416587
C	-1.623919	-1.488235	2.313177
C	1.741240	2.590840	0.857015
C	3.808930	1.652583	-1.417481
C	3.968235	-1.442178	-1.454418
C	1.960092	-2.637310	0.741037
C	1.486845	-0.086825	2.614904
H	-0.140956	-1.600932	-2.155807
H	-2.597723	-1.779298	2.742342
H	-1.048219	-2.408852	2.128912
H	-1.088896	-0.904206	3.071913
H	-3.983512	-2.688945	-0.723852
H	-2.301728	-2.783976	-1.285061
H	-2.698854	-3.223180	0.402761
H	-4.573212	-0.904707	-2.094413
H	-4.557176	0.881852	-2.154800
H	-3.213682	-0.047223	-2.876720
H	-3.729302	2.804548	-1.020451
H	-2.304910	3.325939	-0.070457
H	-2.100308	2.604487	-1.696968
H	-2.502287	2.072624	2.537563
H	-0.979667	1.256006	2.931714
H	-0.969980	2.653347	1.836859
H	0.967537	0.775937	3.052326
H	1.029861	-1.007199	3.003406
H	2.533013	-0.056169	2.963903
H	2.538888	3.295007	0.574571
H	0.813810	2.941804	0.368349
H	1.583704	2.676535	1.946005
H	4.873296	1.365450	-1.462676

H 3.396218 1.540285 -2.436554
H 3.746151 2.716369 -1.143064
H 4.992160 -1.035329 -1.512533
H 4.032021 -2.507890 -1.187289
H 3.528537 -1.372315 -2.465971
H 2.831177 -3.264260 0.494572
H 1.724383 -2.789546 1.808479
H 1.106905 -3.029664 0.155739

21-PH(TS)
C -0.092251 -2.417944 1.590086
Si 0.004787 -1.387351 0.007375
N -1.202998 -0.084490 -0.100295
C -2.681454 -0.059804 -0.020222
C -3.103702 0.319144 1.417607
C 0.103292 -2.478447 -1.534021
Si -0.001190 1.170942 -0.044040
P -0.031933 3.286755 0.113621
N 1.207034 -0.076272 0.071604
C 2.686289 -0.044840 0.008931
C 3.124913 0.362288 -1.416004
C 3.226530 0.972313 1.037195
C 3.234972 -1.448445 0.341923
C -3.237227 0.976340 -1.020966
C -3.228622 -1.458301 -0.376076
H -4.202423 0.332473 1.510102
H -2.698298 -0.408962 2.138581
H -2.718078 1.320026 1.667596
H -4.328786 -1.453518 -0.333786
H -2.918657 -1.745887 -1.393004
H -2.864440 -2.217358 0.336571
H -4.337551 1.003180 -0.962542
H -2.843266 1.978315 -0.791433
H -2.943314 0.707015 -2.048095
H 4.224568 0.382121 -1.494509
H 2.730648 -0.353194 -2.155584
H 2.738898 1.366562 -1.652612
H 4.327241 1.008144 0.989053
H 2.825795 1.976450 0.830977
H 2.925725 0.677344 2.055113
H 4.335483 -1.438195 0.313090
H 2.915410 -1.758169 1.349416
H 2.881872 -2.193743 -0.390216
H 0.778165 -3.089143 1.683015
H -0.111972 -1.760350 2.474031
H -0.998641 -3.046521 1.610050
H 1.001771 -3.118439 -1.523590
H -0.774697 -3.141940 -1.609522
H 0.137792 -1.854485 -2.441792
H 0.120694 3.348178 -1.321793

22-PH(TS)
C -4.320922 -0.326436 0.547858
C -3.419915 -0.080499 1.596353
C -2.046701 0.027335 1.332430
C -1.569365 -0.122691 0.016570

C -2.473261 -0.377927 -1.032080
C -3.846149 -0.473732 -0.766040
C -0.113103 0.001138 -0.257410
N 0.747286 -1.001079 -0.527182
C 0.628896 -2.451836 -0.222375
C 1.976461 -3.081117 -0.633986
N 0.603398 1.143182 -0.227751
Si 2.188810 0.203266 -0.499289
P 3.643849 0.007524 1.060799
C 0.179560 2.563578 -0.260677
C 1.439601 3.376778 -0.626054
C -0.910561 2.797937 -1.328891
C -0.324537 3.001312 1.133197
C 0.398190 -2.654644 1.292224
C -0.506687 -3.102531 -1.040897
H 2.436009 0.385354 -1.973958
H -2.094242 -0.494142 -2.048327
H -4.544088 -0.665001 -1.583347
H -5.390217 -0.404882 0.753642
H -3.784533 0.027759 2.619558
H -1.338143 0.216270 2.139646
H 1.943817 -4.167247 -0.460327
H 2.174861 -2.903027 -1.703141
H 2.801571 -2.661383 -0.037498
H -0.465636 -4.194602 -0.901904
H -1.494079 -2.752693 -0.712195
H -0.385402 -2.881158 -2.112962
H 0.416154 -3.730633 1.530392
H 1.191290 -2.143222 1.858691
H -0.580056 -2.249877 1.592005
H 1.195568 4.449511 -0.644398
H 2.235930 3.209975 0.116217
H 1.814434 3.084157 -1.619578
H -0.506690 4.088123 1.133611
H -1.264894 2.493623 1.389027
H 0.430797 2.767235 1.898499
H -1.122830 3.876617 -1.397714
H -0.563782 2.445555 -2.313068
H -1.843628 2.278325 -1.072324
H 3.432882 1.392073 1.410722

23-PH(TS)
C 4.482230 -0.157792 0.356325
C 3.631928 0.068786 1.450781
C 2.242521 0.107622 1.265153
C 1.697894 -0.089806 -0.018364
C 2.551397 -0.325835 -1.112276
C 3.940361 -0.355148 -0.924437
C 0.224434 -0.018700 -0.205925
N -0.523740 1.101770 -0.158095
C -0.156017 2.534741 -0.145719
C -1.412544 3.302746 -0.611402
N -0.624875 -1.051914 -0.370745
Si -2.101738 0.106455 -0.205133
P -3.281560 -0.083885 1.580053
C -0.420733 -2.498641 -0.111589

C -1.796905 -3.162924 -0.329704
C 0.595587 -3.097588 -1.107900
C 0.037536 -2.729775 1.345921
C -2.760946 0.230706 -1.987446
C 0.206025 2.968744 1.293235
C 1.010118 2.837818 -1.110987
H 2.122208 -0.475254 -2.103981
H 4.598725 -0.531910 -1.777154
H 5.564066 -0.182751 0.501134
H 4.048936 0.214398 2.449103
H 1.572753 0.275573 2.109324
H -1.219184 4.385483 -0.575109
H -1.676545 3.024665 -1.643073
H -2.267630 3.080393 0.047407
H 1.153977 3.928551 -1.163848
H 1.949868 2.383334 -0.771193
H 0.778850 2.466027 -2.121724
H 0.358943 4.059770 1.325082
H -0.606449 2.699987 1.984733
H 1.132957 2.478648 1.622597
H -1.710552 -4.249017 -0.175285
H -2.535401 -2.768929 0.386245
H -2.154167 -2.981248 -1.355940
H 0.086081 -3.811765 1.550722
H 1.036272 -2.301448 1.515908
H -0.680318 -2.262089 2.036539
H 0.619969 -4.191967 -0.983642
H 0.298227 -2.868774 -2.143597
H 1.607964 -2.710038 -0.932037
H -3.403093 -0.641153 -2.201000
H -3.389915 1.128745 -2.103989
H -1.948764 0.260333 -2.734040
H -3.087041 1.319629 1.855766

24-PH(TS)
C -4.800620 -0.142904 -0.062956
C -4.088781 -0.276202 1.140439
C -2.687652 -0.224773 1.138609
C -1.991842 -0.024888 -0.069822
C -2.707878 0.115559 -1.273858
C -4.108341 0.051220 -1.269511
C -0.507491 0.011554 -0.060610
N 0.305918 -1.032425 0.172445
C 0.068736 -2.491638 0.129198
C 1.462072 -3.147401 0.006033
N 0.283943 1.099492 -0.193931
Si 1.797179 0.099122 0.312664
P 2.637761 0.495378 2.243313
C -0.059125 2.538632 -0.044027
C 1.283853 3.297953 -0.104594
C -0.958769 3.006401 -1.208287
C -0.741579 2.803902 1.315996
N 2.739903 -0.073582 -1.133584
C 2.137371 -0.266056 -2.448704
C 4.178778 -0.332085 -1.116735
C -0.605631 -2.964120 1.436933

C -0.787972 -2.880484 -1.095065
H -2.162762 0.265798 -2.206806
H -4.658014 0.153395 -2.207201
H -5.891394 -0.189448 -0.060646
H -4.623268 -0.420967 2.081268
H -2.125461 -0.323729 2.067915
H 1.352822 -4.242333 -0.011972
H 1.962832 -2.821299 -0.917787
H 2.094526 -2.871484 0.864592
H -0.854560 -3.978287 -1.155368
H -1.806330 -2.475934 -1.019956
H -0.322270 -2.506413 -2.020563
H -0.655813 -4.065090 1.451259
H -0.022317 -2.622240 2.305205
H -1.628616 -2.569922 1.514545
H 1.095918 4.381828 -0.067923
H 1.920935 3.027456 0.751759
H 1.820379 3.059490 -1.036060
H -0.892048 3.887894 1.447327
H -1.723327 2.310782 1.365225
H -0.103538 2.427101 2.129891
H -1.075243 4.100582 -1.156202
H -0.499966 2.748649 -2.176248
H -1.957388 2.552892 -1.152508
H 4.698204 0.341114 -1.825986
H 4.571837 -0.158829 -0.103803
H 4.402187 -1.377049 -1.416393
H 2.651690 0.358956 -3.204217
H 2.211499 -1.322422 -2.783259
H 1.076164 0.022680 -2.429762
H 2.597281 -0.913961 2.553949

25-PH(TS)
C -4.307173 -0.238418 -1.711829
C -5.191666 -0.280991 -0.621913
C -4.693427 -0.217244 0.690174
C -3.313464 -0.119912 0.914409
C -2.426379 -0.069957 -0.177924
C -2.926674 -0.126816 -1.492010
C -0.962929 0.014736 0.060792
N -0.180749 1.099592 -0.077887
C -0.563116 2.537345 -0.062720
C -1.303844 2.876021 1.249422
N -0.185991 -0.988428 0.529626
Si 1.287233 0.139148 0.623487
P 2.080617 0.762653 2.511914
C -0.333009 -2.453988 0.336965
C -0.305061 -2.770659 -1.175724
C 0.883507 -3.103688 1.027634
C -1.630213 -2.991370 0.977362
O 2.146232 -0.261382 -0.753806
C 3.575253 -0.212709 -1.033381
C 4.114554 1.208749 -0.790081
C 4.312424 -1.233877 -0.148731
C 3.700858 -0.588973 -2.519129
C 0.761095 3.326495 -0.129994

C -1.428202 2.890948 -1.291161
H -2.231126 -0.082052 -2.331170
H -4.690988 -0.288688 -2.732563
H -6.266618 -0.363783 -0.794072
H -5.379037 -0.248606 1.539129
H -2.913734 -0.085610 1.928665
H 0.830035 -4.196989 0.912227
H 1.818870 -2.748051 0.570459
H 0.897788 -2.858411 2.100503
H -0.333510 -3.861261 -1.331620
H -1.179364 -2.325661 -1.675528
H 0.611865 -2.362987 -1.625869
H -1.617044 -4.092168 0.933629
H -1.695303 -2.682544 2.031926
H -2.523518 -2.637197 0.446725
H 0.545775 4.405455 -0.155926
H 1.378763 3.118258 0.757189
H 1.325462 3.056955 -1.036339
H -1.496012 3.960183 1.298464
H -2.269458 2.350555 1.295202
H -0.683381 2.576854 2.107899
H -1.569582 3.983000 -1.323979
H -0.926054 2.574215 -2.218902
H -2.417748 2.418008 -1.241124
H 4.760402 -0.589387 -2.820693
H 3.282518 -1.592824 -2.693826
H 3.153223 0.134893 -3.142790
H 5.172473 1.265798 -1.094438
H 3.540059 1.937803 -1.383647
H 4.040241 1.467430 0.276978
H 5.388386 -1.231921 -0.388541
H 4.179722 -0.974740 0.912517
H 3.917491 -2.246811 -0.328474
H 1.740997 -0.528822 3.055783

26-PH(TS)
C -4.189610 -0.082821 -1.675765
C -5.049686 -0.156312 -0.568087
C -4.519712 -0.171992 0.732929
C -3.132702 -0.122681 0.927849
C -2.269354 -0.041692 -0.181879
C -2.801839 -0.019190 -1.484561
C -0.800414 0.004355 0.030252
N 0.004364 1.075642 -0.099381
C -0.343490 2.522329 -0.058624
C -1.080325 2.856497 1.256737
N -0.036580 -1.021466 0.470177
Si 1.452608 0.080737 0.578604
P 2.307621 0.654174 2.452905
C -0.222563 -2.482724 0.274418
C -0.362071 -2.782314 -1.235174
C 1.052353 -3.156928 0.822204
C -1.449732 -3.006240 1.049947
O 2.339674 -0.291243 -0.794210
C 3.787941 -0.275132 -0.852018

C 4.226253 -1.461908 -1.715896
C 4.246364 1.070588 -1.424718
C 0.999983 3.280393 -0.109775
C -1.196122 2.918545 -1.282696
H -2.125323 0.049750 -2.337405
H -4.597932 -0.071741 -2.688102
H -6.130225 -0.201265 -0.717747
H -5.185946 -0.226505 1.596003
H -2.709055 -0.146713 1.932608
H 0.967761 -4.248535 0.711415
H 1.936050 -2.812011 0.264726
H 1.190112 -2.917256 1.887721
H -0.418014 -3.870785 -1.397655
H -1.279076 -2.324245 -1.635699
H 0.507585 -2.381583 -1.777069
H -1.472757 -4.105774 0.983556
H -1.381278 -2.719987 2.110738
H -2.388569 -2.616379 0.635368
H 0.810165 4.364398 -0.121629
H 1.608492 3.046603 0.777729
H 1.561693 3.009976 -1.017449
H -1.248998 3.943727 1.321438
H -2.057256 2.351608 1.292744
H -0.469430 2.532437 2.113006
H -1.304484 4.014616 -1.301043
H -0.703228 2.599043 -2.214350
H -2.199585 2.475437 -1.238402
H 4.185251 -0.384689 0.172404
H 5.325697 -1.496589 -1.784068
H 3.871116 -2.409100 -1.280473
H 3.812138 -1.365912 -2.732941
H 5.344621 1.094938 -1.518748
H 3.801204 1.229905 -2.420635
H 3.935260 1.891277 -0.759873
H 1.999667 -0.653502 2.977053

27-PH(TS)
C -2.936899 -0.135088 -1.655383
C -4.249217 -0.159146 -2.151127
C -5.336143 -0.029946 -1.271801
C -5.110074 0.126195 0.106037
C -3.800636 0.152311 0.604939
C -2.710238 0.020314 -0.275306
C -1.314956 0.025380 0.242515
N -0.570559 -1.060873 0.541657
C -0.907003 -2.502787 0.498781
C -2.277003 -2.793651 1.154264
N -0.558516 1.103834 0.496456
Si 0.898944 0.018610 0.978733
P 1.566277 0.171982 3.019280
C -0.831771 2.546176 0.306916
C -1.023174 2.860928 -1.193449
C -2.068012 2.992535 1.119336
C 0.406697 3.288876 0.845429
P 1.978489 -0.022359 -1.086509
C 3.479790 1.172621 -0.980371

C 3.933465 1.632256 0.418344
C 2.890966 -1.706079 -0.987234
C 3.540543 -2.008264 -2.355408
C 3.918578 -1.854201 0.150938
C -0.907974 -2.999345 -0.965021
C 0.179623 -3.237845 1.310914
C 3.245768 2.382344 -1.911832
H -2.084820 -0.229537 -2.330210
H -4.420929 -0.277434 -3.222690
H -6.356989 -0.050101 -1.658386
H -5.953008 0.225837 0.792605
H -3.614678 0.266427 1.673532
H 0.002758 -4.322572 1.254724
H 1.185964 -3.030619 0.919038
H 0.148798 -2.921879 2.363529
H -1.072003 -4.088949 -0.987653
H -1.713717 -2.514784 -1.535057
H 0.052019 -2.774577 -1.452599
H -2.394426 -3.884267 1.255449
H -2.323420 -2.341397 2.156612
H -3.110516 -2.415107 0.549645
H 0.254979 4.374959 0.756042
H 0.579678 3.037260 1.903180
H 1.299695 3.019065 0.264554
H -2.149022 4.090238 1.072499
H -2.994097 2.564138 0.714783
H -1.956995 2.691556 2.172009
H -1.134113 3.948777 -1.331005
H -0.151166 2.513774 -1.768168
H -1.924834 2.367701 -1.584094
H 4.141171 3.028920 -1.923902
H 3.030832 2.061939 -2.943748
H 2.397387 2.997407 -1.568716
H 4.872819 2.207570 0.328434
H 3.186860 2.289233 0.888804
H 4.090252 0.789995 1.103879
H 4.298986 0.576389 -1.418443
H 2.089342 -2.447039 -0.838172
H 4.326750 -2.880968 0.159566
H 4.762175 -1.162802 0.000033
H 3.479540 -1.636249 1.136844
H 4.015753 -3.004968 -2.335473
H 2.797824 -1.988254 -3.168712
H 4.326953 -1.272305 -2.592911
H 1.427035 -1.254493 3.164669

28-PH(TS)
C -5.484905 0.134925 0.534429
C -4.144085 0.538235 0.600942
C -3.137649 -0.258061 0.020786
C -3.484498 -1.457861 -0.628354
C -4.828118 -1.854300 -0.698729
C -5.829369 -1.060883 -0.116829
C -1.716145 0.180073 0.098613
N -1.138055 1.140539 -0.646780
C -1.629626 1.889759 -1.829557

C -2.134007 0.921482 -2.920177
N -0.784520 -0.256587 0.972354
Si 0.408257 1.092274 0.398816
P 0.723187 2.705786 1.794443
C -0.969005 -0.978927 2.259852
C -2.018897 -0.274263 3.148334
C -1.367314 -2.446825 1.996351
C 0.395176 -0.931877 2.977467
P 2.046948 0.271963 -0.914314
Si 1.862082 -1.962315 -1.267813
C 0.053699 -2.373573 -1.715454
Si 3.955865 0.556898 0.298110
C 3.822836 0.007298 2.118478
C 5.300210 -0.501046 -0.558460
C 4.434662 2.391909 0.214819
C -2.748871 2.872078 -1.413520
C -0.432223 2.695298 -2.375273
C 2.979238 -2.385591 -2.757390
C 2.383065 -3.076128 0.195946
H -2.705208 -2.065492 -1.088092
H -5.090967 -2.782813 -1.209281
H -6.874348 -1.372478 -0.170623
H -6.258953 0.753930 0.992053
H -3.866032 1.460398 1.111762
H 0.342859 -1.523294 3.904130
H 1.190382 -1.343986 2.341238
H 0.653518 0.105095 3.239123
H -1.432181 -2.983187 2.956506
H -2.345231 -2.510965 1.498667
H -0.613370 -2.944508 1.367629
H -1.998329 -0.718004 4.156922
H -1.773588 0.796429 3.222247
H -3.032608 -0.393017 2.742695
H -0.766319 3.299153 -3.232755
H -0.036088 3.372762 -1.602498
H 0.377721 2.026262 -2.698852
H -2.989582 3.530812 -2.263533
H -3.663207 2.337010 -1.123754
H -2.410179 3.491985 -0.569591
H -2.432870 1.501759 -3.807506
H -1.331499 0.226169 -3.209721
H -3.002550 0.343879 -2.575604
H 6.278059 -0.314950 -0.079670
H 5.093796 -1.581371 -0.484610
H 5.395805 -0.247089 -1.627170
H 5.382991 2.567769 0.753778
H 4.562644 2.726520 -0.828165
H 3.644994 3.001125 0.684552
H 4.796111 0.144180 2.623490
H 3.077728 0.615935 2.654593
H 3.539652 -1.053369 2.212519
H 2.898160 -3.458920 -3.006523
H 2.688192 -1.805174 -3.648440
H 4.037834 -2.166217 -2.545646
H -0.035894 -3.427914 -2.031327
H -0.589358 -2.218753 -0.837523

H -0.320847 -1.738687 -2.534739
H 2.381398 -4.134719 -0.121117
H 3.397158 -2.837174 0.555137
H 1.693920 -2.983404 1.049853
H 0.210400 3.644083 0.827689

29-PH(TS)
C 3.978899 -0.118887 1.134379
C 4.642464 -0.058329 -0.101851
C 3.903081 0.021508 -1.293265
C 2.501920 0.046971 -1.250900
C 1.835928 -0.019839 -0.012083
C 2.577606 -0.105680 1.181168
C 0.351681 -0.001444 0.030932
N -0.439715 1.077188 -0.172640
C -0.135840 2.527699 -0.055066
C 0.818414 2.980215 -1.181398
N -0.461797 -1.057796 0.219143
Si -1.954182 0.020515 -0.096195
P -3.191665 -0.341408 -1.787868
C -0.195408 -2.513520 0.064638
C 0.839695 -2.994873 1.103263
C -1.543570 -3.218103 0.322039
C 0.286605 -2.815292 -1.371389
Cl -2.692769 0.285078 1.896285
C -1.482490 3.265630 -0.201262
C 0.476230 2.827375 1.330794
H 2.052375 -0.162408 2.135444
H 4.550751 -0.179898 2.062107
H 5.733484 -0.073422 -0.136939
H 4.416114 0.066665 -2.255707
H 1.918059 0.117032 -2.169478
H -1.407870 -4.306922 0.239962
H -1.918044 -2.981601 1.329805
H -2.291883 -2.907147 -0.423987
H 0.900293 -4.093824 1.059861
H 1.838475 -2.587747 0.897966
H 0.531738 -2.700240 2.118377
H 0.403718 -3.903566 -1.499146
H -0.452361 -2.445609 -2.098117
H 1.259087 -2.338460 -1.565054
H -1.312156 4.350746 -0.137104
H -1.944784 3.038303 -1.174123
H -2.177715 2.972130 0.599829
H 0.920335 4.076503 -1.145902
H 1.816499 2.537645 -1.065239
H 0.410247 2.696388 -2.163577
H 0.624895 3.913455 1.439712
H -0.199383 2.480152 2.126874
H 1.451627 2.332096 1.443124
H -2.933614 1.010995 -2.216315

30-PH(TS)
C -4.051405 -0.010506 -1.496381
C -4.891728 -0.081821 -0.372962
C -4.338429 -0.120549 0.918002

C -2.946812 -0.094229 1.087790
C -2.104250 -0.017617 -0.037993
C -2.659032 0.026925 -1.331354
C -0.630500 0.014824 0.139997
N 0.168270 1.093109 0.045947
C -0.158208 2.543496 0.087420
C -0.922972 2.879783 1.386302
N 0.158560 -1.034711 0.473171
Si 1.642118 0.067619 0.545885
P 2.701590 0.483154 2.343511
C -0.075628 -2.495232 0.316121
C -0.408987 -2.820340 -1.156982
C 1.240630 -3.191170 0.719523
C -1.210257 -2.973741 1.247800
Br 2.654238 -0.205418 -1.533522
C 1.194597 3.285796 0.069908
C -0.979585 2.950050 -1.155002
H -1.996924 0.091611 -2.195789
H -4.478265 0.018886 -2.500594
H -5.975414 -0.106810 -0.502831
H -4.989327 -0.173463 1.792704
H -2.506177 -0.132090 2.084855
H 1.119641 -4.280637 0.622192
H 2.067795 -2.872370 0.066547
H 1.499982 -2.956747 1.763404
H -0.513215 -3.910595 -1.277677
H -1.356513 -2.347267 -1.454429
H 0.396104 -2.463828 -1.816899
H -1.263874 -4.073421 1.208389
H -1.007100 -2.668649 2.285957
H -2.183768 -2.570417 0.938854
H 1.014412 4.371460 0.064288
H 1.785288 3.037916 0.965653
H 1.771414 3.019168 -0.829249
H -1.085997 3.968050 1.444252
H -1.903399 2.381308 1.402729
H -0.336302 2.559210 2.260679
H -1.087143 4.046221 -1.167098
H -0.462239 2.636941 -2.075052
H -1.983843 2.506024 -1.137671
H 2.430622 -0.867676 2.768043

31-PH(TS)

C -3.064904 -1.977394 -0.048665
C -2.087576 -1.235117 0.660683
C -2.304580 -0.815572 1.999787
C -3.521512 -1.162788 2.613150
C -4.508521 -1.874956 1.921634
C -4.276981 -2.271375 0.599690
N -0.863623 -0.905963 0.005184
C 0.365184 -1.249435 0.473126
N 0.620481 -2.356634 1.218266
C -0.298567 -3.502478 1.198680
C -1.285842 0.002289 2.794975
C -1.875844 1.343570 3.284386
C -2.834636 -2.475835 -1.475076

C	-3.012919	-4.009826	-1.576464
N	1.247236	-0.333625	-0.004744
Si	-0.153944	0.430050	-1.103094
P	-0.040488	0.021211	-3.214235
C	2.657664	-0.609879	-0.058128
C	3.162185	-1.680138	-0.841455
C	4.531642	-1.991793	-0.729865
C	5.379973	-1.271984	0.115239
C	4.871071	-0.197330	0.855423
C	3.513626	0.156652	0.781928
C	2.303415	-2.505537	-1.794505
C	2.823259	-2.374947	-3.243582
C	2.980931	1.322872	1.615164
C	2.656250	0.914435	3.071243
N	-0.588897	2.030414	-0.496720
Si	-2.272399	2.645708	-0.681068
C	-2.501235	4.172721	0.442257
Si	0.656217	3.309584	-0.700675
C	0.961320	4.141351	0.989206
C	2.240764	2.609232	-1.491261
C	0.168702	4.695977	-1.917619
C	3.941451	2.531073	1.610848
C	2.250028	-3.992778	-1.379892
C	1.816347	-2.548285	2.044386
C	-0.751441	-0.813978	3.993853
C	-3.780935	-1.776927	-2.478599
C	-2.662930	3.085185	-2.493375
C	-3.624601	1.422457	-0.158923
H	-5.042818	-2.830328	0.058374
H	-5.453561	-2.119553	2.411456
H	-3.700402	-0.849671	3.643743
H	4.929969	-2.817002	-1.323435
H	5.537010	0.372383	1.505075
H	-1.803671	-2.231150	-1.770632
H	-3.622565	-2.185720	-3.489487
H	-4.835482	-1.937158	-2.198583
H	-3.591629	-0.694465	-2.520496
H	-2.772565	-4.343787	-2.598591
H	-2.357406	-4.548805	-0.873806
H	-4.052544	-4.304634	-1.358246
H	-0.441269	0.259045	2.143822
H	0.026973	-0.246340	4.529258
H	-1.565060	-1.033083	4.704532
H	-0.322139	-1.771004	3.663066
H	-1.105887	1.909163	3.834706
H	-2.211527	1.951811	2.434460
H	-2.731008	1.182483	3.960728
H	1.282739	-2.099744	-1.807091
H	2.158410	-2.929865	-3.924067
H	2.821646	-1.322001	-3.557736
H	3.844401	-2.781342	-3.339725
H	1.591222	-4.547847	-2.067648
H	3.251109	-4.453731	-1.423886
H	1.863545	-4.115294	-0.357686
H	2.037086	1.639772	1.160656
H	3.454553	3.389035	2.096999

H	4.866587	2.311746	2.167856
H	4.213201	2.816366	0.584375
H	2.358999	1.804861	3.650248
H	1.822448	0.199054	3.113381
H	3.535379	0.463865	3.561406
H	1.498451	-2.958777	3.016638
H	2.516023	-3.250642	1.563456
H	2.330100	-1.602859	2.213506
H	0.305032	-4.419523	1.279097
H	-1.018699	-3.461947	2.031894
H	-0.844005	-3.526329	0.251093
H	1.005226	5.417135	-1.957158
H	0.026854	4.290088	-2.931381
H	-0.737868	5.253763	-1.642993
H	1.883504	4.746701	0.970128
H	0.124781	4.815533	1.233890
H	1.047584	3.414289	1.810915
H	2.995174	3.414970	-1.524752
H	2.705656	1.748904	-0.997111
H	2.020098	2.318341	-2.532250
H	-3.752282	3.039533	-2.669378
H	-2.315618	4.088674	-2.781309
H	-2.171955	2.356955	-3.161474
H	-3.555733	4.495883	0.382582
H	-2.283882	3.939894	1.497435
H	-1.877130	5.032336	0.156699
H	-4.584315	1.935570	-0.351342
H	-3.631540	0.495704	-0.747259
H	-3.603842	1.138371	0.901170
H	6.437022	-1.537188	0.189610
H	-1.406408	-0.431517	-3.136872

32-PH(TS)

C -4.858047 -1.071023 -1.016556
C -3.826880 -0.853333 -0.081642
C -3.937492 -1.401633 1.209992
C -5.061740 -2.163771 1.559783
C -6.082760 -2.384797 0.621977
C -5.979464 -1.835763 -0.666911
C -2.635526 -0.044496 -0.464248
N -1.526835 -0.484076 -1.105499
C -1.265843 -1.768466 -1.782102
C -1.632245 -2.981174 -0.897016
Si -0.928165 1.304817 -1.431071
N -2.477137 1.283221 -0.324920
C -3.286387 2.276565 0.416674
C -3.020917 2.113813 1.930589
Si 0.776671 1.552132 0.237692
P 1.012731 3.329951 1.467970
N 2.355950 1.016194 -0.666243
C 3.308132 1.661874 -1.597043
C 2.587460 2.906388 -2.157270
C 2.524500 -0.014746 0.177045
N 1.444525 -0.043795 0.981856
C 1.087309 -0.906229 2.124443
C -0.428853 -0.707019 2.337810

C 3.696003 -0.929743 0.255523
C 3.811380 -2.021603 -0.624515
C 4.899204 -2.899526 -0.514514
C 5.878409 -2.688047 0.469433
C 5.770501 -1.592773 1.341971
C 4.681623 -0.715441 1.237960
C 4.580061 2.110949 -0.842622
C 3.664688 0.709048 -2.758949
C 1.371756 -2.399035 1.849539
C 1.853238 -0.444392 3.386224
C -2.804286 3.669143 -0.038826
C -4.796422 2.137042 0.115948
C -2.038903 -1.839364 -3.119554
C 0.252776 -1.790790 -2.060847
H 3.044137 -2.182641 -1.382251
H 4.981165 -3.748407 -1.196308
H 6.724974 -3.372408 0.553966
H 6.534589 -1.419524 2.102296
H 4.594300 0.144643 1.902923
H 3.251470 3.425602 -2.865218
H 1.662971 2.620130 -2.682896
H 2.334020 3.602132 -1.341844
H 4.295692 1.242336 -3.488248
H 4.220085 -0.167960 -2.398792
H 2.749152 0.370012 -3.268886
H 5.216914 2.706565 -1.516908
H 4.293628 2.728694 0.022138
H 5.161100 1.245715 -0.493566
H -0.773017 -1.335794 3.173836
H -0.651071 0.344269 2.576381
H -0.972944 -0.981705 1.423464
H 1.492698 -1.001365 4.266933
H 2.930293 -0.635299 3.272285
H 1.696486 0.632052 3.549023
H 0.956908 -2.995322 2.677776
H 0.892718 -2.721776 0.913515
H 2.448310 -2.603573 1.785312
H -3.604455 2.860576 2.493389
H -3.319284 1.109494 2.269029
H -1.952039 2.274543 2.139363
H -5.323715 2.997701 0.557254
H -4.972705 2.138607 -0.971281
H -5.221144 1.218917 0.542872
H -3.379298 4.443588 0.492457
H -1.737019 3.805550 0.201083
H -2.959096 3.794013 -1.122672
H 0.523559 -2.711345 -2.601403
H 0.546813 -0.924040 -2.674864
H 0.806285 -1.749197 -1.112735
H -1.269518 -3.900334 -1.384644
H -1.156404 -2.898231 0.091185
H -2.717142 -3.070920 -0.757906
H -1.759004 -2.750486 -3.674175
H -3.122794 -1.866545 -2.934988
H -1.803516 -0.958694 -3.736852
H -4.782391 -0.624401 -2.008986

H -6.774962 -1.997871 -1.397196
H -6.957278 -2.978995 0.894769
H -5.139409 -2.584931 2.564280
H -3.139886 -1.232704 1.933361
H 0.616585 2.572025 2.631335

33-PH(TS)
C -3.010089 3.182406 0.458056
C -2.202947 2.435616 -0.444170
C -1.580764 3.063815 -1.553552
C -1.741593 4.451957 -1.717593
C -2.511993 5.205044 -0.826157
C -3.147062 4.564819 0.243622
N -1.953945 1.045003 -0.203934
C -2.929488 0.087279 -0.143815
C -4.256301 0.163421 -0.757195
C -4.436550 0.908469 -1.944203
C -5.696040 1.007494 -2.539940
C -6.819019 0.366455 -1.979928
C -6.635882 -0.371340 -0.792560
C -5.381813 -0.477534 -0.186689
C -8.177618 0.448834 -2.643689
C -0.784969 2.288527 -2.603381
C 0.687571 2.753916 -2.660739
C -3.747227 2.558471 1.643569
C -5.277280 2.718236 1.482183
Si -1.004624 0.210556 1.245886
N -2.445135 -0.869010 0.676313
C -3.037939 -2.130054 0.980521
C -3.603786 -2.330202 2.265653
C -4.212467 -3.568057 2.536404
C -4.274272 -4.576254 1.567581
C -3.702253 -4.361281 0.309007
C -3.064308 -3.148962 -0.003654
C -3.583059 -1.255840 3.350217
C -2.660469 -1.685038 4.513408
C -2.418042 -2.965001 -1.370629
C -3.476774 -2.856803 -2.491758
Si 0.911719 -1.053541 0.695597
P 0.848205 -2.916799 1.791230
N 2.311424 0.156998 1.126456
C 2.692642 1.039989 2.182029
C 3.374331 0.485360 3.298411
C 3.793346 1.356869 4.318429
C 3.540711 2.732079 4.250613
C 2.844511 3.252367 3.154989
C 2.399436 2.424027 2.108945
C 3.687170 -1.003716 3.413639
C 3.040816 -1.612610 4.677064
C 1.636934 3.045806 0.945206
C 2.550259 3.987778 0.126825
C 2.872995 0.015095 -0.084721
N 2.089801 -0.851828 -0.791001
C 2.561654 -1.793826 -1.768311
C 3.538895 -2.769529 -1.413628
C 3.863739 -3.758309 -2.360295

C 3.247177 -3.808390 -3.613911
C 2.323926 -2.818367 -3.961558
C 1.985632 -1.788118 -3.066397
C 4.316388 -2.756906 -0.097323
C 5.779438 -2.321484 -0.361347
C 1.075346 -0.665837 -3.559746
C -0.350152 -1.170086 -3.864275
C 4.064161 0.694137 -0.603547
C 4.167378 0.919632 -1.992917
C 5.274155 1.587927 -2.520803
C 6.310654 2.048575 -1.684284
C 6.203507 1.813139 -0.298136
C 5.097897 1.152593 0.243182
C 7.496181 2.797803 -2.254895
C 5.210811 -1.262535 3.394859
C 0.379845 3.799039 1.433366
C 4.289138 -4.116161 0.633234
C 1.668921 -0.001447 -4.826480
C -5.002652 -0.912356 3.854322
C -1.416882 -4.099403 -1.684815
C -1.426549 2.445692 -4.003899
C -3.272630 3.150635 2.989549
H 3.370025 0.575735 -2.646369
H 5.337692 1.757782 -3.598463
H 7.002083 2.152265 0.365925
H 5.040422 0.983816 1.315495
H -5.277488 -1.045061 0.734663
H -7.494933 -0.864939 -0.331278
H -5.812323 1.590728 -3.456954
H -3.582574 1.409472 -2.392121
H 7.313517 3.887267 -2.244231
H 8.407277 2.612083 -1.664702
H 7.688863 2.505517 -3.298919
H -8.279902 1.374467 -3.231756
H -8.333038 -0.400115 -3.333649
H -8.988220 0.417179 -1.898319
H 4.326073 0.942133 5.176589
H 3.877071 3.393588 5.052208
H 2.634461 4.322354 3.103394
H 4.613706 -4.506019 -2.097185
H 3.499504 -4.601161 -4.321651
H 1.866925 -2.826178 -4.953136
H -4.648237 -3.735930 3.523385
H -4.759033 -5.528173 1.795725
H -3.734995 -5.149249 -0.445988
H -1.259201 4.943000 -2.565288
H -2.623321 6.282369 -0.967801
H -3.760119 5.145123 0.936009
H -3.536080 1.483157 1.682990
H -3.822223 2.676780 3.819585
H -2.197525 2.971353 3.137376
H -3.456249 4.236634 3.031613
H -5.796602 2.200312 2.305214
H -5.562633 3.782759 1.513675
H -5.620875 2.293246 0.528258
H -0.802554 1.223894 -2.331065

H -0.864307 1.857314 -4.745700
H -2.473172 2.105112 -4.019561
H -1.409849 3.499795 -4.324454
H 1.210754 2.278268 -3.502647
H 0.745761 3.845369 -2.800012
H 1.223032 2.499798 -1.738509
H -1.853107 -2.023154 -1.337354
H -0.880063 -3.882147 -2.622166
H -0.681835 -4.205091 -0.874284
H -1.939679 -5.061975 -1.807836
H -2.983455 -2.682147 -3.462356
H -4.048390 -3.797207 -2.562954
H -4.183603 -2.036467 -2.303060
H -3.160168 -0.335666 2.925217
H -4.947458 -0.116764 4.615888
H -5.642314 -0.557787 3.029325
H -5.489358 -1.788191 4.313317
H -2.607353 -0.886133 5.271830
H -3.044823 -2.598658 4.996752
H -1.645411 -1.894283 4.140804
H 3.245720 -1.527845 2.557121
H 3.222777 -2.698589 4.698307
H 3.459927 -1.167861 5.595471
H 1.952543 -1.449501 4.673403
H 5.406339 -2.344903 3.466197
H 5.668557 -0.894031 2.462835
H 5.710454 -0.766309 4.243736
H 1.293493 2.233237 0.288231
H 1.981059 4.444543 -0.697340
H 2.931967 4.797007 0.770862
H 3.411179 3.447081 -0.293798
H -0.174444 4.208167 0.576381
H -0.286386 3.118690 1.984285
H 0.654005 4.632987 2.100021
H 3.855961 -2.035453 0.586784
H 4.840659 -4.029008 1.583584
H 3.255199 -4.408412 0.861949
H 4.770799 -4.906728 0.034724
H 6.323317 -2.231383 0.593005
H 6.293553 -3.075481 -0.980300
H 5.827850 -1.356194 -0.885447
H 1.010073 0.091589 -2.767524
H -0.989036 -0.342503 -4.209709
H -0.327381 -1.939958 -4.653039
H -0.804650 -1.611779 -2.971645
H 1.027661 0.830387 -5.157440
H 2.682706 0.391314 -4.650399
H 1.731608 -0.726715 -5.652747
H 0.812176 -3.630011 0.539308

34-PH(TS)
C -5.294436 -1.412358 -0.557329
C -3.943393 -1.532902 -0.145761
C -3.538574 -2.548619 0.760045
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C -5.859255 -3.315681 0.868095

C -6.238005 -2.313520 -0.032026
N -2.978415 -0.572673 -0.600537
Ge -3.091884 1.378995 0.034138
Cl -3.500520 0.965755 2.251623
C -2.092990 -2.711362 1.231401
C -1.538656 -4.113961 0.886398
C -5.749261 -0.345033 -1.551031
C -6.458728 -0.969656 -2.774705
C -2.100657 -0.890684 -1.569186
C -2.337796 -2.143838 -2.391025
C -0.938716 -0.139652 -1.833444
C -0.350275 0.814646 -0.968239
N -1.026856 1.383584 0.044945
C -0.412249 2.378125 0.881161
C -0.317444 3.714794 0.411993
C 0.267418 4.676176 1.256365
C 0.752517 4.329288 2.521935
C 0.642684 3.006375 2.969635
C 0.049034 2.012626 2.170785
C -0.840017 4.144586 -0.958292
C 0.236557 4.885654 -1.785344
C -0.023972 0.567561 2.655914
C -0.378216 0.451077 4.151968
C 1.093053 1.222105 -1.204900
Si 2.345725 0.000113 -2.014475
P 2.575179 -0.302199 -4.125668
N 3.893440 0.427621 -1.055178
C 4.668710 1.656774 -0.755129
C 4.383155 2.122839 0.691071
C 3.845344 -0.747870 -0.405717
N 2.703524 -1.370815 -0.789212
C 2.403028 -2.832336 -0.786296
C 3.406183 -3.576957 -1.695578
C 4.904858 -1.298142 0.480930
C 4.748494 -1.321098 1.879388
C 5.767585 -1.845033 2.688331
C 6.939144 -2.355671 2.105649
C 7.094495 -2.336519 0.709402
C 6.083459 -1.803631 -0.102889
C 6.182644 1.424687 -0.956475
C 4.185486 2.725798 -1.758050
C 2.429586 -3.412335 0.644267
C 0.977944 -2.979486 -1.352268
C -2.098137 5.030704 -0.801192
C 1.311084 -0.149773 2.358587
C -1.975033 -2.468024 2.752955
C -6.663447 0.694079 -0.861192
H 3.831089 -0.937664 2.323784
H 5.643633 -1.857557 3.772935
H 7.728848 -2.767371 2.737254
H 8.002932 -2.733497 0.252346
H 6.197087 -1.775082 -1.187418
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H 0.261688 -2.390837 -0.762738
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H 2.068823 -4.452350 0.605621

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H 1.766178 -2.836892 1.306106
H 3.105269 -4.633089 -1.791423
H 3.423690 -3.110389 -2.692485
H 4.418079 -3.543950 -1.265409
H 4.781371 3.642531 -1.635347
H 4.301783 2.364245 -2.792104
H 3.129431 2.979159 -1.582463
H 6.708746 2.387993 -0.861155
H 6.587232 0.735111 -0.204198
H 6.374379 1.015646 -1.960124
H 4.924479 3.061788 0.889213
H 3.308170 2.303831 0.843390
H 4.722755 1.367371 1.414856
H 1.075882 2.089467 -1.890603
H 1.524407 1.592565 -0.264326
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H 0.342365 5.709163 0.910493
H 1.208753 5.087948 3.161880
H 1.016665 2.741305 3.959572
H -1.134632 3.248862 -1.522703
H -0.149639 5.106548 -2.793357
H 0.511435 5.841623 -1.310907
H 1.153428 4.283787 -1.888900
H -2.483056 5.325780 -1.791652
H -2.892553 4.489678 -0.263809
H -1.856987 5.945179 -0.234570
H -0.814079 0.059187 2.088520
H 1.281142 -1.185422 2.736936
H 1.521026 -0.185028 1.279667
H 2.141734 0.377605 2.858674
H -0.519582 -0.608610 4.413599
H 0.425897 0.850042 4.792741
H -1.309485 0.992294 4.372507
H -7.282214 -2.225260 -0.338772
H -6.605538 -4.005480 1.268426
H -4.219262 -4.211282 1.953688
H -4.861024 0.184268 -1.926988
H -6.952701 1.482464 -1.575900
H -7.581225 0.211078 -0.486418
H -6.152410 1.165298 -0.006745
H -6.731787 -0.181761 -3.495718
H -5.807036 -1.698685 -3.283105
H -7.382324 -1.489745 -2.473305
H -1.469197 -1.959848 0.726846
H -0.479817 -4.184595 1.182484
H -2.098283 -4.894546 1.426866
H -1.608764 -4.332059 -0.190217
H -0.920729 -2.553622 3.066123
H -2.345789 -1.469558 3.017956
H -2.559915 -3.218472 3.309951
H -1.695564 -2.148214 -3.282349
H -2.112340 -3.041944 -1.796736
H -3.394633 -2.214183 -2.691407
H 1.822347 -1.528234 -4.055469

35-PH(TS)
C -2.809793 -2.570159 0.007854
C -3.231825 -1.323037 -0.489607
C -4.461337 -1.217909 -1.167085
C -5.262435 -2.355332 -1.344603
C -4.842729 -3.598093 -0.843082
C -3.615796 -3.703366 -0.167132
C -2.404012 -0.107023 -0.278502
N -2.621214 0.850211 0.634768
C -3.637059 1.002229 1.699087
C -4.962163 1.497791 1.074529
N -1.335495 0.285617 -1.013453
C -0.887239 -0.177288 -2.348665
C -0.505458 -1.671702 -2.330349
Si -1.343904 1.957349 -0.167156
P -2.126876 3.661195 -1.207535
O -0.103340 2.029672 0.917212
Si 1.330110 1.568667 1.700594
N 2.554468 1.270271 0.223980
C 3.497828 2.151993 -0.495169
C 2.717561 3.453555 -0.783744
N 1.514492 -0.327968 1.245188
C 1.238951 -1.533683 2.054602
C 2.315422 -1.729679 3.147768
C 2.575192 -0.050392 0.459852
C 3.630355 -1.005340 0.009278
C 3.430234 -1.780858 -1.148395
C 4.431213 -2.656948 -1.590728
C 5.637035 -2.765995 -0.878799
C 5.839255 -1.995331 0.277541
C 4.840582 -1.115159 0.719528
C -0.129663 -1.273362 2.721681
C 1.136825 -2.804842 1.185128
C -1.981363 0.086454 -3.408030
C 0.372008 0.652356 -2.674494
C -3.868657 -0.309518 2.477597
C -3.085596 2.078221 2.659876
C 4.711727 2.466566 0.411270
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H -2.937768 3.033011 2.130352
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H -4.331105 -1.081447 1.848468
H -2.921210 -0.695981 2.881105
H -5.678946 1.747737 1.873994
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H -5.405919 0.714134 0.442953
H 0.807263 0.310043 -3.626091
H 0.120111 1.719704 -2.770738
H 1.114809 0.543093 -1.871956

H -1.589657 -0.139931 -4.413434
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H -2.291250 1.141547 -3.367827
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H 0.246993 -1.860805 -1.551408
H -1.376568 -2.314567 -2.148871
H 4.568384 2.313547 -2.365774
H 4.632954 0.673716 -1.672739
H 3.136672 1.252710 -2.461735
H 5.366132 3.206461 -0.078387
H 4.367606 2.877176 1.372809
H 5.298002 1.554804 0.600311
H 3.373453 4.174117 -1.296353
H 1.841329 3.252420 -1.417059
H 2.362413 3.911507 0.152735
H -0.448092 -2.158758 3.293916
H -0.066484 -0.416821 3.412187
H -0.885395 -1.041890 1.957761
H 0.828705 -3.651529 1.819785
H 0.385359 -2.668918 0.394126
H 2.098147 -3.057248 0.719080
H 2.026618 -2.554617 3.820063
H 3.287471 -1.975434 2.696061
H 2.417709 -0.807457 3.740282
H 4.992805 -0.511919 1.615631
H 6.774748 -2.077424 0.834649
H 6.416424 -3.448181 -1.224201
H 4.270580 -3.252406 -2.491794
H 2.494859 -1.685479 -1.701263
H -1.420933 3.269867 -2.402273

36-PH(TS)
C 6.946771 -2.374004 -0.281323
C 6.193067 -1.352310 0.326965
C 6.519412 -0.926648 1.628272
C 7.589514 -1.519218 2.315299
C 8.345321 -2.530548 1.701608
C 8.023954 -2.955115 0.401329
C 5.032791 -0.737059 -0.380335
N 3.858660 -1.338319 -0.617034
C 3.181316 -2.429679 0.119463
C 3.955230 -3.763573 0.027996
Si 3.214467 0.132055 -1.686237
N 4.979021 0.498668 -0.912165
C 6.105030 1.379868 -1.312304
C 5.505875 2.478989 -2.217201
O 2.320022 0.859238 -0.364381
C 1.075916 1.412843 -0.346500
C 0.043387 0.876989 -1.131785
C -1.266325 1.385904 -1.074383
C -1.566924 2.521806 -0.293177
C -0.503054 3.007920 0.502679
C 0.803405 2.496341 0.537051
O -2.251310 0.706228 -1.781421
Si -2.664146 -0.872317 -1.312588
P -1.834209 -2.654725 -2.147545

C 1.877086 3.074068 1.485559
C 1.338974 4.243818 2.342714
C -2.920103 3.269875 -0.208212
C -3.997411 2.805416 -1.216476
N -4.517134 -0.767040 -1.247251
C -5.623640 -0.780954 -2.231336
C -4.993895 -0.336830 -3.568885
C -4.494924 -0.819489 0.092794
N -3.193076 -0.754494 0.473789
C -2.568517 -1.188338 1.756050
C -1.076032 -0.813334 1.657258
C -5.674308 -0.967809 0.982938
C -6.219932 0.158847 1.627140
C -7.342735 0.014018 2.452960
C -7.920663 -1.252357 2.642747
C -7.374335 -2.376369 2.002973
C -6.254394 -2.236153 1.170254
C -6.167718 -2.221705 -2.367275
C -6.756234 0.191742 -1.842110
C -3.179338 -0.469434 2.976864
C -2.724629 -2.718715 1.909166
C 6.728679 2.042887 -0.063188
C 7.184765 0.613666 -2.110946
C -3.507634 3.095513 1.215613
C -2.687654 4.783242 -0.479572
C 2.373792 1.972862 2.461549
C 3.083756 3.610197 0.671273
C 2.994305 -2.017429 1.598022
C 1.797827 -2.602432 -0.539268
H -5.763990 1.137676 1.475263
H -7.765872 0.889945 2.948480
H -8.794564 -1.362468 3.287892
H -7.819181 -3.362342 2.150231
H -5.821918 -3.102659 0.668741
H -5.765744 -0.322925 -4.353142
H -4.555429 0.667066 -3.474614
H -4.204129 -1.042347 -3.875099
H -7.504658 0.197335 -2.650025
H -7.254159 -0.117557 -0.913710
H -6.366932 1.212692 -1.717679
H -6.892050 -2.265645 -3.196800
H -5.339415 -2.916402 -2.572313
H -6.679037 -2.532254 -1.444355
H -0.563775 -1.121128 2.581961
H -0.597480 -1.330353 0.813192
H -0.951140 0.270030 1.519435
H -2.169851 -3.063285 2.797072
H -3.784912 -2.984673 2.037764
H -2.336285 -3.229509 1.015518
H -2.602915 -0.759318 3.869693
H -3.111549 0.621636 2.861773
H -4.226920 -0.751514 3.141638
H 0.236232 0.019153 -1.776448
H -0.731473 3.848984 1.152743
H -3.648783 5.320654 -0.411928
H -1.994986 5.237870 0.243941

H -2.274543 4.931670 -1.489825
H -4.447447 3.667035 1.314196
H -3.717731 2.031488 1.399617
H -2.806419 3.446944 1.988763
H -4.876490 3.465375 -1.112864
H -3.634327 2.867524 -2.252419
H -4.311355 1.773333 -1.029464
H 2.147285 4.607880 2.996350
H 1.001080 5.084527 1.715219
H 0.499325 3.925341 2.982129
H 3.823171 4.064539 1.354091
H 3.569230 2.795621 0.122027
H 2.756331 4.381474 -0.045302
H 3.117934 2.400512 3.156238
H 1.533423 1.577792 3.056143
H 2.838768 1.146421 1.910283
H 6.682195 -2.705332 -1.286318
H 8.609114 -3.741977 -0.078833
H 9.181037 -2.988307 2.234781
H 7.832436 -1.189887 3.327515
H 5.927762 -0.138002 2.095565
H 7.929934 1.325891 -2.500834
H 7.706789 -0.119747 -1.481419
H 6.723581 0.089934 -2.963592
H 7.471589 2.793621 -0.378682
H 5.948011 2.544586 0.528107
H 7.235436 1.299594 0.567334
H 6.299021 3.184030 -2.510498
H 5.070296 2.039291 -3.127742
H 4.720727 3.037861 -1.686776
H 3.334413 -4.568716 0.453429
H 4.171697 -4.008339 -1.023558
H 4.899846 -3.726159 0.586821
H 2.437660 -2.801427 2.137157
H 3.970244 -1.883474 2.089087
H 2.430975 -1.075397 1.654408
H 1.237012 -3.396262 -0.023787
H 1.217421 -1.671835 -0.470202
H 1.892565 -2.875607 -1.601113
H -1.049077 -2.845246 -0.957038

37-PH(TS)
C -5.286602 -0.415358 1.748633
C -5.121088 -0.244836 0.360859
C -6.236673 -0.344944 -0.490819
C -7.506452 -0.614857 0.040900
C -7.667615 -0.785500 1.425286
C -6.555688 -0.684737 2.277990
C -3.762699 0.034499 -0.182570
N -3.200914 1.246901 -0.355140
C -3.836110 2.585362 -0.333176
C -2.680513 3.607499 -0.367899
Si -1.850101 0.493455 -1.540428
N -2.878154 -0.874546 -0.634212
C -3.058258 -2.317389 -0.916468
C -1.640443 -2.887313 -1.120086

P 0.006134 0.914908 -0.204667
Si -0.163383 0.459884 1.994587
C -0.997256 -1.208535 2.397619
Si 1.676479 -0.136904 -1.256911
P 1.430963 -1.060940 -3.190211
N 2.812076 -1.051806 -0.040474
C 3.066566 -2.504292 0.188359
C 1.713716 -3.211596 -0.009731
C 3.732507 -0.066418 -0.140246
N 3.222920 0.886289 -0.938270
C 3.580852 2.323338 -1.057854
C 2.682452 2.908244 -2.167498
C 5.084737 -0.055292 0.479937
C 6.222229 -0.317026 -0.307636
C 7.496862 -0.301440 0.274269
C 7.643667 -0.011096 1.640909
C 6.511104 0.258508 2.425614
C 5.232428 0.232066 1.849710
C 4.075673 -3.043889 -0.850554
C 3.566698 -2.762287 1.625380
C 3.293292 3.034248 0.283603
C 5.060054 2.517113 -1.458703
C 1.557508 0.543088 2.821532
C -1.282795 1.803734 2.759913
C -3.746137 -3.077666 0.239303
C -3.876539 -2.490269 -2.218116
C -4.715988 2.761563 -1.594494
C -4.694641 2.833360 0.927894
H -6.105533 -0.212505 -1.565503
H -1.113032 -2.362546 -1.933363
H -1.702063 -3.956251 -1.377671
H -1.058203 -2.775921 -0.196216
H -2.041142 3.497856 0.519133
H -3.091172 4.629068 -0.396026
H -2.056848 3.454991 -1.262835
H -3.219731 -2.906440 1.190081
H -3.709565 -4.155442 0.013600
H -4.798398 -2.788975 0.357359
H -8.656107 -0.996225 1.838503
H -4.416443 -0.338122 2.402864
H -8.368187 -0.691694 -0.625326
H -4.118653 2.576739 -2.500346
H -5.118676 3.787228 -1.634846
H -5.561682 2.057948 -1.573903
H 2.858089 2.385634 -3.120090
H 2.917647 3.975766 -2.298253
H 1.620143 2.811794 -1.899446
H 0.963379 -2.798344 0.678057
H 1.826325 -4.287166 0.194610
H 1.357226 -3.089137 -1.042887
H -4.901459 -2.112785 -2.082639
H -3.931738 -3.557447 -2.489448
H -3.395178 -1.939202 -3.040232
H -5.597093 2.209107 0.942630
H -5.008450 3.889622 0.930361
H -4.118219 2.644977 1.845173

H 3.740031 -2.762316 -1.860752
H 4.129433 -4.142420 -0.775836
H 5.081558 -2.638791 -0.669246
H 8.374838 -0.511362 -0.339715
H 6.097725 -0.527016 -1.370339
H 2.235890 2.903335 0.557721
H 3.508555 4.110964 0.187493
H 3.930880 2.621505 1.080777
H 5.746285 2.247414 -0.645792
H 5.219655 3.579117 -1.704632
H 5.299796 1.912583 -2.346598
H -6.677572 -0.817001 3.355027
H 4.347100 0.429974 2.454581
H 4.548158 -2.303535 1.803076
H 3.661955 -3.849429 1.777753
H 2.849550 -2.370058 2.363005
H -0.383128 -2.078039 2.116555
H -1.946616 -1.277727 1.845205
H -1.213048 -1.283626 3.478986
H 6.621098 0.486390 3.487714
H 8.637808 0.005343 2.092174
H 1.474522 0.382624 3.911482
H 2.028196 1.525883 2.654182
H 2.221256 -0.228081 2.403801
H -2.279088 1.755503 2.295029
H -0.882015 2.817113 2.593752
H -1.398478 1.652110 3.848183
H 1.911443 0.132241 -3.839711

38-PH(TS)
C 6.528566 -0.028061 -1.780488
C 5.829122 -0.098160 -0.560616
C 6.529454 -0.370808 0.629187
C 7.917476 -0.570412 0.600067
C 8.611611 -0.506374 -0.619601
C 7.914909 -0.236563 -1.809846
C 4.354956 0.120104 -0.532306
N 3.738653 1.309309 -0.555994
C 4.222504 2.633677 -0.127304
C 4.489529 2.611309 1.397186
Si 2.004393 0.489920 -0.832759
N 3.394857 -0.828732 -0.552858
C 3.502446 -2.241962 -0.987953
C 3.594546 -2.302402 -2.530139
C 1.483512 0.669877 1.020911
C 0.566620 1.671919 1.525284
C 0.526154 1.606572 2.958966
C 1.406219 0.547709 3.368005
C 1.983810 -0.022014 2.183092
Fe -0.063096 -0.171763 2.143689
C -0.655230 -2.031158 1.522090
C -1.567450 -1.031080 1.011704
C -2.096565 -0.335043 2.166076
C -1.534285 -0.910709 3.354769
C -0.640939 -1.962124 2.953850
Si -2.107941 -0.881731 -0.776198

N -3.947804 -1.250520 -0.628051
C -4.738403 -2.376800 -0.069454
C -5.202857 -2.051927 1.368336
N -3.065872 0.725567 -0.803324
C -2.791330 2.132022 -1.187386
C -1.369705 2.146276 -1.782473
C -4.233056 0.065632 -0.660679
C -5.584210 0.678035 -0.590917
C -6.484324 0.522313 -1.662966
C -7.746932 1.128948 -1.612579
C -8.122377 1.883772 -0.488249
C -7.230192 2.032454 0.586514
C -5.961998 1.435871 0.534337
C -2.839688 3.016864 0.079750
C -3.781994 2.656215 -2.250228
P -1.035783 -1.522485 -2.518870
C 4.708728 -2.971230 -0.353579
C 2.205534 -2.929978 -0.517752
C 3.089560 3.635637 -0.435823
C 5.497809 3.070372 -0.885325
C -5.951342 -2.702026 -0.969159
C -3.793609 -3.597002 -0.037658
H 5.978432 -0.433215 1.569146
H 8.455850 -0.779705 1.526871
H 9.691749 -0.665693 -0.642907
H 8.451910 -0.185868 -2.759467
H 5.980398 0.193383 -2.697673
H 2.216047 -3.988420 -0.824251
H 2.129749 -2.877718 0.579974
H 1.320560 -2.448583 -0.967335
H 4.606208 -4.050088 -0.552405
H 5.667309 -2.636571 -0.770744
H 4.725190 -2.817484 0.737114
H 3.622845 -3.351848 -2.867765
H 2.718426 -1.809031 -2.977485
H 4.511663 -1.799096 -2.876357
H 3.397668 4.648331 -0.132291
H 2.860097 3.639256 -1.512805
H 2.178773 3.365738 0.119640
H 5.727247 4.117925 -0.629589
H 6.363848 2.452091 -0.614766
H 5.338962 3.000809 -1.972975
H 4.776529 3.617246 1.746734
H 3.586495 2.284638 1.932964
H 5.311606 1.916045 1.627173
H -6.180204 -0.060018 -2.533292
H -8.436522 1.014071 -2.451178
H -9.107195 2.353671 -0.449703
H -7.520701 2.612233 1.464817
H -5.266146 1.541560 1.367497
H -6.422292 -3.633844 -0.616408
H -6.703454 -1.902359 -0.932991
H -5.625054 -2.843776 -2.011076
H -5.738356 -2.919613 1.786825
H -4.332585 -1.829869 2.004024
H -5.885197 -1.189067 1.374348

H -4.340811 -4.472171 0.344977
H -3.421103 -3.823119 -1.048628
H -2.934981 -3.403958 0.623271
H -2.496497 4.035511 -0.164003
H -3.866238 3.081398 0.470065
H -2.186203 2.597557 0.859462
H -1.075902 3.180980 -2.018270
H -0.639039 1.731629 -1.072761
H -1.326059 1.539846 -2.698924
H -3.435751 3.643468 -2.595358
H -3.807156 1.973156 -3.113193
H -4.798706 2.769724 -1.851190
H -2.781507 0.509473 2.128286
H -1.702014 -0.569835 4.375237
H -0.015433 -2.555440 3.618271
H -0.062581 -2.697257 0.902062
H -0.007574 2.362957 0.912429
H -0.100458 2.208235 3.615607
H 1.555989 0.202573 4.390201
H 2.665520 -0.868567 2.148017
H -1.654738 -2.820680 -2.360962

39-PH(TS)
C -3.567697 -2.047632 0.744764
C -3.583518 -1.062744 -0.260453
C -4.625107 -1.045676 -1.208678
C -5.644209 -2.006259 -1.148228
C -5.622463 -2.993550 -0.149465
C -4.582954 -3.013522 0.794454
C -2.515816 -0.030723 -0.342009
N -2.370857 1.049641 0.450335
C -3.366323 1.737165 1.313398
C -4.581034 2.171979 0.463984
N -1.548373 0.034543 -1.281495
C -0.952088 -1.032644 -2.124066
C -0.459723 -2.187607 -1.225102
Si -0.942725 1.661484 -0.616358
P -1.238130 3.482263 -1.725766
Si 0.936592 1.264133 0.751287
N 2.533243 1.180773 0.020720
C 3.522482 2.154631 -0.478451
C 2.782892 3.477166 -0.759302
N 1.505447 -0.352382 1.252883
C 1.243410 -1.075084 2.510734
C 1.711571 -0.287885 3.761450
C 2.901630 0.009993 0.861446
C 3.697836 -1.073898 0.148990
C 3.177181 -1.741650 -0.972008
C 3.931494 -2.719356 -1.631689
C 5.223733 -3.040647 -1.178053
C 5.752121 -2.378928 -0.059503
C 4.987760 -1.401616 0.598823
C -0.283406 -1.280603 2.585817
C 1.938129 -2.454394 2.480547
C 4.633777 2.411557 0.567484
C 4.158968 1.632007 -1.789052

C -1.964791 -1.548895 -3.168327
C 0.234265 -0.371891 -2.858240
C -3.810028 0.834668 2.484392
C -2.648857 2.982693 1.874870
H -2.764999 -2.050037 1.481575
H -4.562384 -3.779649 1.571896
H -6.413852 -3.744451 -0.106615
H -6.452356 -1.984620 -1.881795
H -4.627428 -0.279007 -1.984435
H -3.324954 3.519670 2.557151
H -1.744199 2.691808 2.432397
H -2.364260 3.667969 1.061105
H -4.449777 1.421678 3.162234
H -4.385431 -0.031375 2.132459
H -2.936202 0.476602 3.050506
H -5.270573 2.770523 1.081179
H -4.236308 2.776197 -0.388778
H -5.125364 1.291938 0.089867
H 0.754543 -1.123321 -3.471221
H -0.124529 0.434130 -3.516847
H 0.958659 0.054829 -2.146174
H -1.446382 -2.229037 -3.862905
H -2.785173 -2.102562 -2.692903
H -2.382416 -0.708888 -3.744255
H 0.079863 -2.930984 -1.833714
H 0.215675 -1.800914 -0.446840
H -1.314751 -2.689471 -0.746397
H 4.880087 2.368291 -2.182061
H 4.684987 0.682030 -1.617683
H 3.375882 1.465682 -2.545047
H 5.322766 3.187980 0.198398
H 4.194487 2.754311 1.518464
H 5.218463 1.497962 0.756481
H 3.475914 4.207785 -1.205554
H 1.938608 3.325351 -1.450250
H 2.383498 3.905268 0.175264
H -0.557407 -1.794632 3.520993
H -0.812550 -0.313516 2.553801
H -0.617726 -1.886280 1.730843
H 1.665737 -3.031762 3.379241
H 1.634494 -3.015417 1.583914
H 3.032111 -2.344205 2.456640
H 1.472111 -0.846176 4.681614
H 2.800629 -0.124423 3.738683
H 1.214908 0.694278 3.805214
H 0.790038 2.239136 1.903616
H 5.392836 -0.882728 1.472597
H 6.754811 -2.621875 0.299613
H 5.813439 -3.801312 -1.694682
H 3.515971 -3.231856 -2.502994
H 2.181626 -1.481518 -1.319365
H 3.492012 0.324628 1.748126
H -0.858956 2.791422 -2.934135

40-PH(TS)
C -4.676393 1.741234 0.888034

C -3.542661 1.279720 0.198088
C -3.063105 2.016612 -0.897859
C -3.694422 3.203288 -1.287202
C -4.820904 3.668077 -0.584174
C -5.314152 2.932328 0.503784
C -2.847707 0.012383 0.665116
N -2.467009 -0.964364 -0.394642
C -3.459577 -1.819141 -1.078481
C -4.244299 -0.985977 -2.117912
N -1.461872 0.205016 1.196868
C -1.189225 0.823716 2.506541
C -1.271250 2.364624 2.392285
Si -0.934942 -1.269741 0.400038
Cl -1.012569 -2.982776 1.718782
Si 1.044524 -1.570047 -0.868864
P 1.454837 -3.255025 -2.128008
N 2.390838 -0.976488 0.293592
C 3.416950 -1.676031 1.116161
C 2.769236 -2.996284 1.577742
C 2.485755 0.184143 -0.387949
N 1.550009 0.151710 -1.358781
C 0.961110 1.251581 -2.163519
C -0.199337 0.617298 -2.958869
C 3.476442 1.271400 -0.164081
C 3.312491 2.192458 0.887610
C 4.256592 3.210932 1.079675
C 5.371096 3.308434 0.230957
C 5.537975 2.388025 -0.816312
C 4.590607 1.374625 -1.019011
C 4.657407 -1.981866 0.247199
C 3.805130 -0.839165 2.353237
C 0.433491 2.358448 -1.225306
C 1.997896 1.822701 -3.154935
C -2.175791 0.329991 3.591879
C 0.244438 0.420966 2.908097
C -2.682459 -2.934922 -1.804210
C -4.449497 -2.452089 -0.071487
H 2.449057 2.108762 1.547685
H 4.121901 3.925741 1.893596
H 6.107544 4.099378 0.385488
H 6.403547 2.459484 -1.477543
H 4.707209 0.659914 -1.834592
H 3.489006 -3.558279 2.191800
H 1.867700 -2.803624 2.177103
H 2.493418 -3.621261 0.713986
H 4.470642 -1.442596 2.990376
H 4.337874 0.079015 2.073212
H 2.910625 -0.571969 2.935101
H 5.373453 -2.585092 0.828421
H 4.352873 -2.542617 -0.649226
H 5.158059 -1.051528 -0.059049
H -0.701901 1.392328 -3.557310
H 0.182641 -0.159316 -3.639596
H -0.942018 0.159886 -2.285786
H 1.495884 2.542251 -3.821275
H 2.808735 2.345744 -2.631144

H 2.426212 1.014564 -3.767393
H -0.125676 3.106981 -1.808427
H -0.234587 1.925346 -0.467462
H 1.267797 2.867889 -0.721100
H -4.960650 -1.633720 -2.649204
H -4.801712 -0.171116 -1.634789
H -3.553160 -0.545298 -2.853079
H -5.124728 -3.146546 -0.596816
H -3.903587 -3.007106 0.706258
H -5.069770 -1.679230 0.410723
H -3.382162 -3.559315 -2.381414
H -1.939907 -2.509594 -2.496474
H -2.151099 -3.581604 -1.089042
H 0.555276 0.971081 3.810126
H 0.305279 -0.658421 3.117387
H 0.944400 0.651856 2.091555
H -1.053719 2.826632 3.369850
H -0.540222 2.731259 1.655346
H -2.272991 2.680888 2.070221
H -1.888684 0.736284 4.575254
H -3.200648 0.667566 3.373043
H -2.167513 -0.769444 3.643928
H -5.058123 1.162130 1.733608
H -6.193731 3.281109 1.049460
H -5.313864 4.594014 -0.888668
H -3.314073 3.767024 -2.142648
H -2.202331 1.639251 -1.441859
H -3.492099 -0.465106 1.428851
H 1.017999 -2.480145 -3.263925

41-PH(TS)

C	-3.740052	0.361477	-1.763965
C	-3.467630	-0.183924	-0.495662
C	-4.483142	-0.862324	0.205614
C	-5.761297	-0.984727	-0.355396
C	-6.028499	-0.446569	-1.625693
C	-5.015810	0.222860	-2.330676
C	-2.113079	-0.037973	0.102112
N	-1.565506	1.068243	0.584060
C	-2.245399	2.275765	1.081616
C	-3.353009	1.953343	2.102310
Si	0.001642	-0.020626	1.249304
P	-0.082618	-0.185279	3.401565
N	1.567477	-1.068047	0.552888
C	2.242912	-2.287426	1.028033
C	3.377810	-1.990779	2.025744
C	2.114417	0.052155	0.099911
N	1.231782	1.058504	0.328200
C	1.072163	2.305823	-0.438704
C	0.773052	2.004780	-1.920384
C	3.470855	0.214062	-0.487765
C	3.764861	-0.343631	-1.746132
C	5.045413	-0.197449	-2.299760
C	6.042337	0.491882	-1.591527
C	5.754064	1.043391	-0.331580
C	4.470725	0.913606	0.215742

C	2.707638	-3.182231	-0.138294
C	2.247091	3.289659	-0.279882
N	-1.234418	-1.053191	0.303499
C	-1.081152	-2.287015	-0.485607
C	-0.712338	-1.958051	-1.945524
C	-2.289880	-3.238047	-0.400654
C	-2.747833	3.173653	-0.066517
H	0.182933	2.776853	-0.000647
H	1.453213	-2.817173	1.585033
H	2.987108	-0.888029	-2.283944
H	5.264754	-0.625561	-3.279929
H	7.041351	0.598969	-2.019027
H	6.528452	1.576649	0.223394
H	4.233878	1.341526	1.190508
H	0.557369	2.936917	-2.468277
H	1.641515	1.518648	-2.393165
H	-0.097391	1.336171	-2.000283
H	1.956304	4.267841	-0.696880
H	2.497889	3.422143	0.783517
H	3.142273	2.942161	-0.813827
H	3.755961	-2.936729	2.447041
H	4.214007	-1.473194	1.532040
H	2.984190	-1.368615	2.843888
H	3.021112	-4.164201	0.252108
H	1.893311	-3.337492	-0.864124
H	3.563374	-2.730861	-0.661648
H	-1.450657	2.816544	1.621121
H	-3.722717	2.887807	2.555937
H	-4.200095	1.447184	1.615004
H	-2.937127	1.308090	2.891354
H	-3.071203	4.145862	0.339948
H	-1.950332	3.351024	-0.806007
H	-3.604749	2.712483	-0.578866
H	-0.225047	-2.795102	-0.023062
H	-2.007459	-4.214793	-0.826339
H	-2.591698	-3.385783	0.647173
H	-3.150293	-2.853827	-0.965779
H	-0.511730	-2.882560	-2.511926
H	-1.542877	-1.425196	-2.435994
H	0.185998	-1.323123	-1.971170
H	-2.950482	0.892197	-2.298506
H	-5.219112	0.641552	-3.318359
H	-7.023483	-0.548259	-2.063798
H	-6.547835	-1.502746	0.196868
H	-4.262125	-1.281812	1.187707
H	0.917070	0.849979	3.530484

42-PH(TS)

C	-3.160011	-1.786153	2.334019
C	-2.108348	-2.230278	1.306084
C	-2.552918	-3.456670	0.480465
N	-1.547820	-1.113831	0.505214
C	-2.126317	0.026785	0.070919
N	-3.408203	0.189904	-0.411180
C	-4.175498	1.397615	0.007065
C	-4.877724	1.171192	1.362394

Si	0.047709	-0.135478	1.031396
N	1.820928	1.061827	0.292347
C	2.700175	2.170133	0.673827
C	2.662121	3.280864	-0.397480
P	0.214896	-0.144669	3.185885
N	-1.179130	1.006402	0.198221
C	-0.928097	2.231856	-0.589868
C	-1.155816	3.506546	0.249078
N	1.243508	-1.056622	-0.012616
C	0.853857	-1.885855	-1.186996
C	1.778832	-3.068913	-1.504375
C	-1.623207	2.307066	-1.958411
C	-3.989202	-0.906197	-1.232669
C	-5.325923	-1.475644	-0.724495
C	-4.091906	-0.523611	-2.729076
C	-5.169957	1.941245	-1.034492
C	2.260343	-0.115269	-0.098856
N	3.561389	-0.484923	-0.485329
C	4.421735	-1.217347	0.493147
C	3.885062	-2.601411	0.901600
C	4.222367	0.257442	-1.588128
C	5.457928	1.107711	-1.211698
C	4.615554	-0.742362	-2.700048
C	2.299607	2.741855	2.044479
C	0.638132	-0.989020	-2.423618
C	4.697450	-0.374849	1.759322
H	-1.231199	-2.543672	1.897365
H	0.150457	2.177380	-0.785331
H	-2.581263	-4.336555	1.143626
H	-3.558155	-3.343357	0.048027
H	-1.838276	-3.663328	-0.332026
H	-3.469191	-2.653129	2.941140
H	-2.706400	-1.036647	3.000630
H	-4.051521	-1.360619	1.858653
H	-0.679464	4.365632	-0.251989
H	-2.223347	3.747677	0.377503
H	-0.706494	3.384087	1.244016
H	-1.157466	3.121498	-2.536466
H	-1.499105	1.371694	-2.522402
H	-2.693528	2.525614	-1.877341
H	-0.122502	-2.299457	-0.907929
H	0.233329	-1.574826	-3.265440
H	-0.067105	-0.181490	-2.180069
H	1.587954	-0.531665	-2.744482
H	1.364206	-3.622079	-2.363967
H	2.789596	-2.727989	-1.759434
H	1.842287	-3.753613	-0.647647
H	3.730372	1.801473	0.754787
H	3.030673	3.513875	2.338827
H	1.303169	3.205737	1.997158
H	2.251626	1.950425	2.804395
H	3.365801	4.084634	-0.125099
H	2.939087	2.899285	-1.392145
H	1.653255	3.717778	-0.459401
H	3.452718	0.931081	-1.992425
H	5.096378	-0.217701	-3.542117

H	5.329716	-1.485962	-2.309848
H	3.730599	-1.276096	-3.073744
H	5.869440	1.561976	-2.127202
H	5.218783	1.916399	-0.510120
H	6.247094	0.481565	-0.767962
H	5.374169	-1.378031	-0.035395
H	5.320872	-0.948211	2.464523
H	5.225423	0.557328	1.513570
H	3.749426	-0.125557	2.261686
H	4.538119	-3.014656	1.686837
H	2.863709	-2.523056	1.298101
H	3.885328	-3.295100	0.052408
H	-3.244368	-1.705635	-1.182171
H	-3.425573	2.175711	0.168910
H	-5.570505	2.892553	-0.651557
H	-4.698090	2.132183	-2.006860
H	-6.019838	1.263446	-1.190730
H	-5.364410	2.106540	1.684471
H	-5.646758	0.387976	1.290223
H	-4.145409	0.877921	2.126835
H	-5.613741	-2.321573	-1.369486
H	-5.248093	-1.844538	0.305339
H	-6.135516	-0.734612	-0.769499
H	-4.248991	-1.442834	-3.317030
H	-4.932687	0.152574	-2.933660
H	-3.161725	-0.047569	-3.071000
H	1.321642	-1.067448	3.095407

43-PH(TS)

C -2.859338 -0.013793 -0.305910
P -1.661207 1.221721 -0.082563
C -1.180113 2.147770 -1.626646
Si -4.666180 0.273246 -0.622149
C -5.456976 -1.246468 -1.470325
P -2.028273 -1.506084 0.178523
C -2.884802 -2.328498 1.613073
C -5.633299 0.591526 0.998178
C -4.895118 1.805867 -1.746918
C -2.237622 -2.815451 -1.150759
C -2.124233 2.622305 1.052570
Si -0.009283 -0.045402 0.923418
P 0.127221 -0.233606 3.078524
P 1.660359 -1.210815 -0.153486
C 2.142987 -2.650926 0.923337
P 2.008657 1.512024 0.240541
C 2.886990 2.257460 1.705605
C 1.175369 -2.069818 -1.733400
C 2.840776 0.047917 -0.327702
Si 4.650022 -0.219275 -0.645281
C 5.434455 1.321187 -1.461558
C 5.619280 -0.563936 0.968114
C 4.890556 -1.726693 -1.802200
C 2.222688 2.884173 -1.025552
H -5.965027 2.009614 -1.927549
H -4.465043 2.716382 -1.293004
H -4.410417 1.661040 -2.727482

H -6.708087 0.764258 0.808807
H -5.546453 -0.268166 1.684658
H -5.240874 1.474377 1.532001
H -6.526625 -1.066235 -1.676558
H -4.963293 -1.483961 -2.427483
H -5.395523 -2.143846 -0.830228
H 6.502819 1.146948 -1.679562
H 4.933493 1.582504 -2.408686
H 5.376967 2.201846 -0.798422
H 6.695320 -0.725156 0.775294
H 5.526336 0.280518 1.672405
H 5.232553 -1.459639 1.484108
H 5.962492 -1.926421 -1.975170
H 4.455668 -2.647271 -1.373999
H 4.417357 -1.559765 -2.784962
H -2.392212 2.207295 2.034427
H -1.274081 3.313725 1.169592
H -2.983855 3.174159 0.639643
H -2.091767 2.552836 -2.093781
H -0.487867 2.970864 -1.397279
H -0.698898 1.452348 -2.330362
H -1.718843 -3.743361 -0.855858
H -3.303582 -3.043516 -1.307741
H -1.810828 -2.448213 -2.095440
H -2.494225 -3.349202 1.760358
H -2.669544 -1.736748 2.515880
H -3.972795 -2.381103 1.442745
H 2.475161 3.255222 1.933725
H 2.714578 1.595235 2.567915
H 3.968127 2.353597 1.511844
H 1.715659 3.802165 -0.682367
H 3.289321 3.109426 -1.181983
H 1.784408 2.567785 -1.983447
H 0.492634 -2.909471 -1.537003
H 0.683473 -1.347717 -2.401993
H 2.087674 -2.443847 -2.223969
H 3.026313 -3.158724 0.503324
H 2.379098 -2.273123 1.928278
H 1.311894 -3.370954 0.993231
H -0.806276 0.849993 3.269734

44-PH(TS)
C 3.200643 1.045215 -0.395246
C 2.755855 -0.382263 -0.030984
C 3.301731 -0.747254 1.368254
C 3.313183 -1.353653 -1.098973
N 1.257818 -0.483923 0.008533
Si -0.000016 0.750399 -0.176266
P -0.000016 2.842250 0.231964
C 0.681817 -1.739889 0.184941
C -0.681798 -1.739904 0.184936
N -1.257815 -0.483949 0.008527
C -2.755847 -0.382280 -0.030978
C -3.313182 -1.353701 -1.098936
C -3.301720 -0.747225 1.368272
C -3.200604 1.045198 -0.395290

H 1.304905 -2.623597 0.285289
H -1.304872 -2.623627 0.285242
H 4.406098 -1.234560 -1.157424
H 3.100893 -2.406141 -0.858497
H 2.879144 -1.123196 -2.083992
H 4.301711 1.070800 -0.407959
H 2.832541 1.328321 -1.393661
H 2.826836 1.783221 0.326236
H 4.402173 -0.701696 1.360845
H 2.922215 -0.037567 2.118860
H 2.998050 -1.764739 1.659908
H -4.301671 1.070837 -0.407915
H -2.826702 1.783228 0.326119
H -2.832567 1.328220 -1.393756
H -4.402159 -0.701609 1.360882
H -2.998087 -1.764725 1.659924
H -2.922152 -0.037552 2.118865
H -4.406075 -1.234478 -1.157526
H -2.878999 -1.123397 -2.083927
H -3.101051 -2.406191 -0.858326
H -0.000264 3.188758 -1.166321

45-PH(TS)
C -3.339087 -1.022158 -0.558616
C -2.662562 0.184767 -0.284223
C -3.353560 1.339637 0.147565
C -4.747838 1.265107 0.291795
C -5.456063 0.079574 0.025792
C -4.735510 -1.048459 -0.399390
N -1.235755 0.244724 -0.455461
C -0.683284 0.934641 -1.536919
C 0.683355 0.934607 -1.536909
N 1.235787 0.244659 -0.455448
Si -0.000016 -0.362434 0.644520
P -0.000195 -1.874962 2.124399
C -2.606150 2.616629 0.472634
C -6.958779 0.017016 0.218460
C -2.586366 -2.257987 -1.004511
C 2.662592 0.184712 -0.284191
C 3.353601 1.339634 0.147450
C 4.747878 1.265111 0.291692
C 5.456099 0.079547 0.025819
C 4.735538 -1.048533 -0.399224
C 3.339112 -1.022251 -0.558437
C 2.606227 2.616697 0.472325
C 2.586386 -2.258135 -1.004168
C 6.958814 0.017015 0.218489
H -1.337903 1.403756 -2.267210
H 1.338008 1.403703 -2.267181
H -5.271289 -1.976881 -0.615304
H -5.291055 2.153024 0.627702
H -3.285612 3.365272 0.906369
H -1.792876 2.420652 1.191971
H -2.133059 3.055643 -0.421507
H -1.852984 -2.018884 -1.791422
H -2.029380 -2.696122 -0.158510

H -3.282578 -3.018664 -1.389082
H -7.444238 0.948863 -0.114481
H -7.398352 -0.822706 -0.342118
H -7.215750 -0.122847 1.283506
H 5.291099 2.153065 0.627497
H 5.271313 -1.976981 -0.615034
H 3.282612 -3.018935 -1.388470
H 2.029249 -2.696048 -0.158150
H 1.853130 -2.019167 -1.791237
H 2.133667 3.055924 -0.421996
H 1.792562 2.420760 1.191227
H 3.285600 3.365174 0.906487
H 7.398332 -0.823033 -0.341641
H 7.444316 0.948658 -0.114966
H 7.215803 -0.122275 1.283608
H -0.000095 -0.912152 3.194439

46-PH(TS)
C -3.348128 1.343931 0.169581
C -2.662725 0.185523 -0.262563
C -3.335662 -1.025218 -0.536342
C -4.733017 -1.053452 -0.377394
C -5.435136 0.083827 0.042566
C -4.744534 1.272604 0.315011
N -1.235448 0.244181 -0.433215
Si -0.000002 -0.362578 0.667453
P 0.000030 -1.869720 2.151744
C -2.578030 -2.260074 -0.976526
C -2.594736 2.616732 0.496869
C -0.683227 0.933276 -1.515555
C 0.683219 0.933273 -1.515558
N 1.235440 0.244177 -0.433219
C 2.662717 0.185522 -0.262568
C 3.348126 1.343944 0.169529
C 4.744532 1.272615 0.314969
C 5.435128 0.083823 0.042575
C 4.733005 -1.053467 -0.377348
C 3.335651 -1.025232 -0.536303
C 2.594749 2.616776 0.496736
C 2.578015 -2.260098 -0.976451
H 6.519903 0.043149 0.160939
H -6.519912 0.043156 0.160921
H 1.337706 1.401082 -2.246763
H -1.337714 1.401088 -2.246758
H 5.286792 2.158682 0.653652
H 5.268171 -1.982221 -0.588330
H 3.271266 -3.023473 -1.360879
H 2.022498 -2.694715 -0.127694
H 1.843291 -2.021389 -1.762134
H 1.780107 2.415689 1.213023
H 3.270334 3.366285 0.934904
H 2.123061 3.057311 -0.397366
H -5.268188 -1.982195 -0.588412
H -5.286791 2.158661 0.653728
H -3.270335 3.366266 0.934971
H -1.780176 2.415600 1.213237

H -2.122932 3.057253 -0.397178
H -1.843343 -2.021353 -1.762242
H -2.022466 -2.694684 -0.127796
H -3.271288 -3.023456 -1.360928
H -0.000025 -0.903192 3.218279

47-PH(TS)
C -3.466447 -1.176184 -0.231700
C -2.647387 -0.027798 -0.324604
C -3.165860 1.283177 -0.199149
C -4.546085 1.422713 0.030672
C -5.378321 0.301355 0.132248
C -4.840306 -0.984664 0.002964
N -1.230782 -0.183403 -0.529691
C -0.683769 -0.114874 -1.812693
C 0.683625 -0.114931 -1.812743
N 1.230732 -0.183474 -0.529780
Si 0.000015 -0.306581 0.715275
P 0.000172 -0.049998 2.813925
C -2.271975 2.520957 -0.256235
C -2.774182 3.550397 -1.292465
C -2.889223 -2.586494 -0.323912
C -2.822105 -3.222766 1.084776
C 2.647374 -0.028034 -0.324810
C 3.166161 1.282945 -0.200578
C 4.546395 1.422366 0.029224
C 5.378350 0.300896 0.131965
C 4.840033 -0.985108 0.003867
C 3.466145 -1.176524 -0.230740
C 2.272468 2.520829 -0.258690
C 2.151382 3.158834 1.145365
C 2.888693 -2.586815 -0.321792
C 3.682817 -3.486357 -1.294474
C 2.822243 -3.222269 1.087291
C 2.775609 3.550117 -1.294610
C -2.151978 3.158715 1.148014
C -3.683945 -3.485443 -1.296650
H -6.447244 0.429813 0.316547
H 6.447285 0.429273 0.316245
H -1.342547 -0.080978 -2.676914
H 1.342347 -0.081081 -2.677009
H -5.491789 -1.856105 0.090707
H -4.967234 2.423791 0.141995
H -1.263612 2.212616 -0.568302
H -1.860776 -2.513558 -0.707631
H 4.967795 2.423437 0.139640
H 5.491290 -1.856631 0.092494
H 1.860050 -2.513989 -0.705011
H 1.264344 2.212538 -0.571577
H -3.193628 -4.468750 -1.382420
H -4.711720 -3.654155 -0.936868
H -3.742301 -3.033012 -2.299457
H -2.374454 -4.229346 1.030182
H -2.221343 -2.602271 1.768465
H -3.834821 -3.315751 1.510383
H -2.079996 4.405493 -1.338683

H -2.844978 3.101545 -2.296219
H -3.769007 3.937792 -1.019281
H -1.461965 4.018573 1.117921
H -3.135795 3.516827 1.493604
H -1.776804 2.426696 1.880035
H 3.192585 -4.469799 -1.379186
H 3.740354 -3.034622 -2.297643
H 4.710889 -3.654634 -0.935339
H 2.374374 -4.228795 1.033510
H 3.835169 -3.315209 1.512407
H 2.221959 -2.601249 1.770924
H 1.461396 4.018692 1.114594
H 1.775688 2.426996 1.877301
H 3.134952 3.516998 1.491611
H 2.081356 4.405110 -1.341677
H 3.770093 3.937728 -1.020502
H 2.847476 3.101099 -2.298212
H -0.000096 -1.475083 3.023698

48-PH(TS)
C -3.214513 0.751361 -0.998462
C -2.735252 -0.337027 -0.014926
N -1.261127 -0.545211 -0.189585
C -0.691446 -1.846501 0.211777
C 0.802356 -1.829537 -0.163556
N 1.293904 -0.441090 -0.036043
C 2.774156 -0.257709 0.009149
C 3.166868 1.206809 -0.260783
C -3.506614 -1.639695 -0.326989
C -3.022617 0.097216 1.441819
Si -0.024209 0.674327 -0.142682
P -0.152669 2.777943 0.152473
C 3.274390 -0.662253 1.416873
C 3.452450 -1.144419 -1.064593
H -1.185757 -2.680988 -0.306134
H 1.366509 -2.507169 0.496146
H -4.107731 0.197363 1.608675
H -2.633499 -0.652155 2.151056
H -2.543441 1.067574 1.643072
H -4.299149 0.900893 -0.874508
H -2.703781 1.705579 -0.804500
H -3.016448 0.439110 -2.036519
H -4.584964 -1.423223 -0.300561
H -3.250471 -2.015768 -1.330423
H -3.302395 -2.429264 0.412788
H 4.264290 1.288549 -0.208713
H 2.836885 1.522413 -1.262582
H 2.717631 1.890572 0.471131
H 4.536397 -0.953502 -1.055842
H 3.296153 -2.217249 -0.875005
H 3.061324 -0.901010 -2.065151
H 4.371868 -0.577308 1.466245
H 2.833254 0.001017 2.176402
H 3.003127 -1.702917 1.655912
H 0.936200 -2.180757 -1.202782
H -0.817040 -2.001818 1.302192

H -0.178118 2.994987 -1.272907

49-PH(TS)
C -3.247241 1.294859 -0.081497
C -2.821541 -0.184658 -0.104061
N -1.339759 -0.318151 -0.185508
C -0.807442 -1.650867 -0.544130
C 0.664783 -1.728586 -0.077229
C 0.760612 -2.235423 1.377043
C -3.478682 -0.861503 -1.332384
C -3.310532 -0.866069 1.197204
Si -0.044141 0.820399 -0.066424
P 0.050513 2.871051 0.494747
N 1.213022 -0.360484 -0.237703
C 2.692205 -0.110975 -0.217214
C 3.016271 1.002139 -1.240582
C 3.144601 0.344566 1.191206
C 3.472571 -1.378329 -0.628882
H -0.872238 -1.800636 -1.637145
H -4.408769 -0.805415 1.264547
H -3.026995 -1.929969 1.228434
H -2.874732 -0.359179 2.071839
H -4.346116 1.341561 -0.016946
H -2.813069 1.829235 0.773875
H -2.922400 1.811264 -0.997230
H -4.568372 -0.712955 -1.287747
H -3.100469 -0.411205 -2.263579
H -3.284958 -1.944700 -1.359100
H 4.103617 1.179680 -1.262906
H 2.683850 0.701884 -2.247299
H 2.516972 1.941339 -0.959775
H 4.544532 -1.132433 -0.653955
H 3.330365 -2.204606 0.084065
H 3.172715 -1.719496 -1.632686
H 4.227165 0.554315 1.189727
H 2.607568 1.262254 1.474437
H 2.942699 -0.434835 1.941062
H 1.195200 -2.427511 -0.739933
H -1.393897 -2.447213 -0.059836
H 0.345914 -3.255047 1.449846
H 1.802296 -2.258930 1.724908
H 0.185251 -1.571778 2.042107
H 0.187665 3.242550 -0.892338

50-PH(TS)
C 3.417265 -1.302023 0.726728
C 2.908855 -0.365175 -0.385484
N 1.428841 -0.463947 -0.533064
C 0.848952 0.049559 -1.790704
C -0.681657 0.245780 -1.610569
C -1.037577 1.714242 -1.254768
C -0.463043 2.214299 0.079174
C -0.875904 3.661295 0.402150
C -0.293795 4.139764 1.744043
C 3.600992 -0.771588 -1.710238
C 3.279198 1.094614 -0.028734

Si 0.195953 -1.106682 0.487967
P 0.184428 -1.703378 2.532143
N -1.112203 -0.725659 -0.579108
C -2.564130 -1.029426 -0.369249
C -2.700907 -2.511406 0.051502
C -3.153541 -0.130812 0.744820
C -3.364410 -0.836631 -1.676045
H 1.050726 -0.658466 -2.613637
H 4.373727 1.202709 0.040154
H 2.915663 1.798152 -0.794725
H 2.835054 1.367269 0.940610
H 4.512994 -1.208394 0.792565
H 2.972392 -1.054855 1.699672
H 3.165405 -2.348841 0.494881
H 4.691685 -0.755260 -1.563873
H 3.301796 -1.790506 -2.002678
H 3.359464 -0.081841 -2.533216
H -3.766040 -2.760184 0.184022
H -2.276140 -3.167239 -0.725523
H -2.180691 -2.693705 1.003670
H -4.405542 -1.142614 -1.494599
H -3.373595 0.211118 -2.011447
H -2.955031 -1.464395 -2.483581
H -4.214756 -0.381493 0.908499
H -2.603377 -0.297222 1.683240
H -3.086893 0.932989 0.473504
H -1.163855 0.006392 -2.569954
H 1.312261 1.013763 -2.058490
H -0.664612 2.349626 -2.078907
H -2.133598 1.827456 -1.244101
H -0.814730 1.558478 0.893924
H 0.636157 2.140860 0.064747
H -0.540820 4.328951 -0.411942
H -1.978608 3.725787 0.427600
H -0.598427 5.174322 1.970376
H -0.635865 3.492809 2.568887
H 0.808557 4.103932 1.725085
H 0.208677 -3.093090 2.150994

51-PH(TS)
C -3.400466 0.672213 -1.025829
C -2.856873 -0.314017 0.029425
N -1.366415 -0.399292 -0.099025
C -0.687700 -1.598285 0.406175
C 0.806073 -1.551012 -0.032647
C 1.565223 -2.461193 0.955364
C -3.499235 -1.695833 -0.230617
C -3.224802 0.170054 1.451403
Si -0.229523 0.903785 -0.128066
P -0.600420 2.992643 0.093310
N 1.193102 -0.091222 -0.000761
C 2.629342 0.362969 0.037354
C 2.759174 1.829601 -0.439598
C 3.158464 0.300618 1.493334
C 3.550319 -0.462351 -0.895193
C 0.882432 -2.117555 -1.474531

H -1.132701 -2.519118 0.002030
H -4.319408 0.189299 1.581112
H -2.800717 -0.508044 2.210560
H -2.829988 1.184654 1.612296
H -4.498911 0.715314 -0.951494
H -2.997163 1.681307 -0.860745
H -3.126858 0.332978 -2.038080
H -4.592364 -1.575298 -0.260526
H -3.166574 -2.107082 -1.197272
H -3.261667 -2.419151 0.564929
H 3.829807 2.088916 -0.457495
H 2.352389 1.950169 -1.455702
H 2.234211 2.529482 0.221178
H 4.571765 -0.061502 -0.805008
H 3.591052 -1.528870 -0.645105
H 3.232468 -0.356843 -1.943227
H 4.160738 0.757007 1.539705
H 2.485719 0.867935 2.154592
H 3.237657 -0.728516 1.865934
H -0.762638 -1.647903 1.511869
H 1.086432 -3.454478 0.938794
H 2.622583 -2.600004 0.701043
H 1.495136 -2.062937 1.977555
H 0.537766 -3.164949 -1.472165
H 0.217957 -1.535366 -2.131136
H 1.897156 -2.093313 -1.884838
H -0.722744 3.146024 -1.334859

52-PH(TS)
C 0.703749 3.757354 -0.456247
C 1.417330 2.554036 -0.533373
C 0.714911 1.339168 -0.606965
C -0.714814 1.339222 -0.606981
C -1.417135 2.554152 -0.533433
C -0.703457 3.757409 -0.456289
N 1.251224 0.050521 -0.735310
Si -0.000029 -1.144988 -0.974123
P -0.000313 -3.246925 -1.212595
N -1.251206 0.050613 -0.735296
C -2.692558 -0.231202 -0.661527
C -3.249282 -0.456781 0.776258
C -2.473613 -1.587481 1.482083
C 2.692569 -0.231351 -0.661563
C 3.249301 -0.456955 0.776211
C 3.174395 0.825568 1.629451
C 2.473652 -1.587689 1.482001
C 4.727794 -0.874707 0.609155
C -3.174373 0.825770 1.629449
C -4.727772 -0.874537 0.609216
H -2.505639 2.555520 -0.527455
H -1.249180 4.700589 -0.394055
H 1.249545 4.700488 -0.393969
H 2.505834 2.555307 -0.527317
H 2.867603 -1.149767 -1.242558
H 3.243728 0.587372 -1.152239
H 5.190794 -1.033935 1.596027

H 4.809563 -1.812019 0.034585
H 5.301924 -0.092812 0.083438
H 3.582575 0.627051 2.634187
H 3.764967 1.639285 1.177168
H 2.136837 1.173169 1.739493
H 2.942514 -1.813586 2.453537
H 1.430196 -1.288227 1.675413
H 2.460246 -2.504550 0.872536
H -2.867648 -1.149616 -1.242511
H -3.243700 0.587537 -1.152196
H -3.582408 0.627257 2.634243
H -2.136836 1.173482 1.739335
H -3.765095 1.639408 1.177218
H -5.190790 -1.033691 1.596090
H -5.301882 -0.092666 0.083441
H -4.809534 -1.811883 0.034700
H -2.942422 -1.813306 2.453661
H -2.460273 -2.504395 0.872691
H -1.430138 -1.288021 1.675417
H 0.000014 -3.064071 -2.644656

53-PH(TS)
C -0.011561 3.601857 -0.385550
C 1.371904 3.321278 -0.371269
C 1.797212 1.985410 -0.447650
C 0.857102 0.945179 -0.532775
C -0.540200 1.243090 -0.540476
C -0.964949 2.580081 -0.465295
C 2.385570 4.442944 -0.247402
N 1.113079 -0.426532 -0.658472
C 2.468904 -0.994931 -0.647919
C 3.025789 -1.375722 0.755323
C 4.412933 -2.013138 0.515690
N -1.334615 0.096058 -0.672480
C -2.804041 0.131785 -0.665621
C -3.470873 0.012238 0.736330
C -4.996558 -0.012269 0.492197
Si -0.363885 -1.350866 -0.800573
P -0.778202 -3.303486 -1.499589
C -3.043688 -1.299284 1.426370
C -3.114308 1.208634 1.641165
C 3.178437 -0.140106 1.665016
C 2.103773 -2.405644 1.438860
H -2.027140 2.818968 -0.472014
H -0.346352 4.640453 -0.331703
H 2.862467 1.758164 -0.438720
H 2.436601 -1.907612 -1.263067
H 3.152102 -0.283380 -1.139044
H 4.872326 -2.296759 1.476219
H 4.327916 -2.918911 -0.107052
H 5.089293 -1.304313 0.008499
H 3.555049 -0.448839 2.654137
H 3.894596 0.581263 1.239003
H 2.215949 0.373654 1.805431
H 2.557194 -2.746919 2.383806
H 1.123423 -1.961643 1.679657

H 1.935361 -3.280539 0.791376
H -3.146653 -0.714805 -1.280729
H -3.136098 1.060918 -1.156270
H -3.589508 1.085323 2.628248
H -2.026847 1.287890 1.786623
H -3.473631 2.155815 1.206876
H -5.534195 -0.078378 1.451592
H -5.327322 0.905478 -0.023108
H -5.283302 -0.879644 -0.124975
H -3.612020 -1.434779 2.361068
H -3.221745 -2.169022 0.774319
H -1.972461 -1.278768 1.687169
H 3.369566 4.137613 -0.637213
H 2.059047 5.338197 -0.800963
H 2.525435 4.743364 0.806754
H -0.893558 -3.793472 -0.149375

54-PH(TS)
C -0.555090 3.728074 -0.489770
C 0.843395 3.602765 -0.506094
N 1.491531 2.421548 -0.556229
C 0.729279 1.324543 -0.593676
C -0.703826 1.332219 -0.582031
C -1.351501 2.572173 -0.526970
N 1.257558 0.034534 -0.681629
C 2.711266 -0.209279 -0.655208
C 3.302209 -0.467948 0.760496
C 4.825585 -0.642632 0.566952
N -1.252103 0.052775 -0.667535
C -2.701338 -0.199201 -0.659403
C -3.337477 -0.401378 0.746972
C -4.828320 -0.729074 0.506631
Si -0.003104 -1.174578 -0.773916
P -0.046667 -3.175569 -1.448010
C -2.666402 -1.582139 1.477152
C -3.223292 0.871450 1.609916
C 3.033427 0.721741 1.703710
C 2.717617 -1.757014 1.371611
H -2.438469 2.634514 -0.510526
H -1.016634 4.715744 -0.446991
H 1.478644 4.492221 -0.478144
H 2.906058 -1.089006 -1.287355
H 3.199685 0.669246 -1.100086
H 5.311108 -0.840014 1.536157
H 5.043756 -1.488920 -0.105799
H 5.272680 0.268732 0.136450
H 3.517965 0.542331 2.677919
H 3.418942 1.658815 1.276551
H 1.953372 0.849836 1.876483
H 3.211764 -1.975485 2.332594
H 1.638087 -1.650126 1.572989
H 2.855354 -2.618532 0.699206
H -2.868098 -1.113562 -1.249590
H -3.203582 0.634397 -1.177104
H -3.676564 0.695126 2.599041
H -2.172265 1.160676 1.759278

H -3.752133 1.717322 1.140350
H -5.345920 -0.874085 1.468206
H -5.330070 0.092034 -0.032849
H -4.937327 -1.651976 -0.086376
H -3.192017 -1.786255 2.424134
H -2.685312 -2.493955 0.859673
H -1.615928 -1.352870 1.721219
H -0.081739 -3.666383 -0.094428

55-PH(TS)
C -1.565388 -1.448628 -0.808835
C -1.063795 -0.124786 -0.750229
C -1.980721 0.944518 -0.711415
C -3.362813 0.700356 -0.725776
C -3.852754 -0.640636 -0.776326
C -2.937879 -1.709401 -0.820145
C 0.395910 0.134731 -0.721896
C 0.949491 1.284353 -1.337559
C 2.322174 1.546243 -1.301560
C 3.184828 0.644430 -0.655676
C 2.648877 -0.547024 -0.078061
C 1.266353 -0.772252 -0.084594
N 3.638608 -1.368317 0.479543
Si 5.220387 -0.630821 0.367769
P 7.207270 -1.275873 0.700183
N 4.572730 0.744234 -0.495871
C 5.347497 1.915150 -0.937986
C 5.444199 3.093149 0.077570
C 4.074825 3.756206 0.329203
N -4.398617 1.637488 -0.720595
C -4.126144 3.079653 -0.650390
C -4.057458 3.689663 0.782357
C -3.742674 5.192371 0.606753
N -5.246574 -0.692171 -0.812404
C -5.965149 -1.973238 -0.825619
C -6.327946 -2.560846 0.572273
C -7.029308 -3.913275 0.314000
Si -6.033756 0.917904 -0.848018
C -5.417090 3.536458 1.492944
C -2.955929 3.030452 1.636963
C 3.347291 -2.689911 1.059160
C 3.286495 -3.879046 0.051850
C 2.072297 -3.784949 -0.895173
C 4.580087 -3.947956 -0.783123
C 3.157735 -5.159664 0.908598
C 6.030029 2.605724 1.417589
C 6.403608 4.127535 -0.554374
C -5.075162 -2.787522 1.441919
C -7.299255 -1.619065 1.311836
H -1.607011 1.963042 -0.632044
H -0.864256 -2.282125 -0.876288
H -3.293933 -2.737234 -0.869750
H -6.906962 -1.821858 -1.378802
H -5.375594 -2.712346 -1.392533
H -7.321830 -4.380948 1.267892
H -7.939115 -3.776091 -0.294466

H -6.358386 -4.608770 -0.218060
H -5.373125 -3.175410 2.430052
H -4.395033 -3.520263 0.979310
H -4.519254 -1.849958 1.588825
H -7.606469 -2.069224 2.270015
H -6.825520 -0.648161 1.528479
H -8.204769 -1.432544 0.710706
H -4.933178 3.597390 -1.194837
H -3.187539 3.296153 -1.186759
H -2.963893 3.461837 2.651630
H -3.113085 1.945088 1.719404
H -1.957739 3.200641 1.203296
H -3.695240 5.689975 1.588739
H -2.772063 5.334407 0.101985
H -4.521929 5.691687 0.006466
H -5.388035 4.035959 2.475218
H -6.228328 3.988619 0.898123
H -5.663172 2.475369 1.657306
H 0.858256 -1.653788 0.403924
H 2.720303 2.444981 -1.769267
H 0.290130 1.970945 -1.870699
H 4.149410 -2.901510 1.782440
H 2.400684 -2.630407 1.621462
H 3.085125 -6.045367 0.257447
H 4.035177 -5.285185 1.564183
H 2.253417 -5.123674 1.539881
H 4.559679 -4.841124 -1.428829
H 4.675264 -3.062869 -1.432639
H 5.471387 -3.993826 -0.139275
H 2.065303 -4.655130 -1.572072
H 1.125703 -3.788006 -0.329415
H 2.107245 -2.871792 -1.506073
H 6.368541 1.560045 -1.143194
H 4.921235 2.278393 -1.887383
H 6.504184 5.004097 0.105482
H 7.405737 3.693967 -0.706613
H 6.022829 4.474787 -1.529973
H 6.195970 3.464922 2.087881
H 5.334906 1.914876 1.922344
H 6.985444 2.079494 1.267676
H 4.189161 4.579899 1.053133
H 3.659664 4.177555 -0.601065
H 3.349431 3.036388 0.735117
H 7.082994 -0.959392 2.101998

56-PH(TS)
C 4.438707 1.694315 -1.724879
C 4.163124 1.366383 -0.382878
C 4.723308 2.145516 0.651154
C 5.544375 3.239191 0.343445
C 5.812230 3.564909 -0.995919
C 5.259111 2.790151 -2.027778
P 2.994195 -0.005869 0.001285
C 1.321341 0.432403 -0.037349
C 0.687383 1.740815 0.103325
C -0.763788 1.672595 0.156317

C -1.496016 2.877498 0.305223
C -0.853341 4.116361 0.392109
C 0.550277 4.181872 0.321769
C 1.304372 3.012537 0.178548
C -1.311061 0.316044 0.049122
P -3.012979 -0.001779 0.006943
C -3.431992 -1.682100 -0.557971
C -3.122756 -2.780634 0.272065
C -3.451089 -4.078798 -0.148075
C -4.072081 -4.285047 -1.387184
C -4.364552 -3.192022 -2.222392
C -4.044982 -1.891270 -1.810631
C 3.595967 -0.656123 1.617600
C 2.656927 -1.030213 2.594360
C 3.092290 -1.552428 3.821448
C 4.463772 -1.705754 4.076409
C 5.406417 -1.326783 3.106166
C 4.975192 -0.799529 1.880260
C 3.342708 -1.285945 -1.271562
C 4.322961 -2.279475 -1.089404
C 4.611289 -3.175852 -2.127378
C 3.937816 -3.079156 -3.355725
C 2.969596 -2.079910 -3.544442
C 2.671258 -1.185498 -2.507873
Si 0.058418 -0.891219 -0.095295
P 0.354277 -2.994776 0.283400
C -3.835685 0.179171 1.642337
C -5.062180 -0.460382 1.915502
C -5.668098 -0.304630 3.171114
C -5.051348 0.484647 4.155515
C -3.823024 1.111482 3.888046
C -3.209601 0.956921 2.636405
C -3.890781 1.145709 -1.132029
C -3.184677 1.627869 -2.252032
C -3.828774 2.460514 -3.177579
C -5.173880 2.817944 -2.987157
C -5.875422 2.344918 -1.866670
C -5.236450 1.510174 -0.937427
H 2.387973 3.091639 0.126259
H 1.060452 5.146619 0.383354
H -1.445754 5.026587 0.513339
H -2.585414 2.845176 0.363085
H -5.526296 -1.092520 1.156007
H -6.614740 -0.806330 3.383222
H -5.522877 0.602213 5.133626
H -3.337141 1.715887 4.656814
H -2.249198 1.429265 2.424897
H -2.133157 1.363112 -2.374099
H -3.277149 2.839600 -4.040242
H -5.672392 3.471157 -3.706639
H -6.918695 2.628649 -1.712442
H -5.778230 1.154015 -0.059966
H -2.639575 -2.627817 1.234822
H -3.196779 -4.926176 0.490283
H -4.324355 -5.298259 -1.708139
H -4.844056 -3.350934 -3.190439

H -4.274856 -1.042560 -2.455615
H 4.833235 -2.377733 -0.131680
H 5.355525 -3.959577 -1.970909
H 4.162346 -3.783425 -4.159613
H 2.435392 -2.004436 -4.493966
H 1.895614 -0.428232 -2.633223
H 4.509949 1.900905 1.692058
H 5.971056 3.838260 1.150588
H 6.450442 4.418348 -1.234288
H 5.467753 3.036436 -3.070929
H 4.017399 1.090759 -2.529953
H 5.708377 -0.487833 1.134136
H 6.474830 -1.436770 3.304198
H 4.799855 -2.115535 5.031451
H 2.357646 -1.844473 4.574370
H 1.594055 -0.905396 2.387980
H 0.415459 -3.347534 -1.112045

57-PH(TS)
C -4.749182 1.399140 1.658978
C -4.316100 0.157118 1.153114
C -4.861718 -1.032302 1.672724
C -5.827580 -1.005100 2.693491
C -6.251152 0.245372 3.184783
C -5.716811 1.436404 2.672781
P -2.986264 0.052840 -0.123242
C -3.505727 -1.324640 -1.211847
C -4.359119 -1.124819 -2.311226
C -4.803815 -2.232010 -3.045506
C -4.411332 -3.528716 -2.683127
C -3.563668 -3.743486 -1.579122
C -3.126029 -2.630044 -0.844039
C -3.086785 -5.135768 -1.216917
C -6.386309 -2.295255 3.261205
C -1.384283 -0.218817 0.470526
Si -0.070337 -0.698732 -0.718724
P -0.230534 -0.985055 -2.851341
C -0.791838 0.401989 1.652983
C 0.657789 0.487165 1.606820
C 1.334577 1.106203 2.689625
C 0.637505 1.611533 3.791714
C -0.763808 1.493503 3.851468
C -1.462566 0.893954 2.798876
C 1.249664 -0.078193 0.392171
P 2.949257 -0.010320 0.057307
C 3.501451 1.678026 -0.421756
C 4.683937 1.884174 -1.157638
C 5.052940 3.189316 -1.520046
C 4.249252 4.277327 -1.152157
C 3.059210 4.085575 -0.420166
C 2.693043 2.775733 -0.066554
C 2.191385 5.263679 -0.021870
C 3.488460 -1.104352 -1.295011
C 4.169777 -2.305343 -1.009835
C 4.583351 -3.160816 -2.043111
C 4.305341 -2.785134 -3.375135

C 3.619995 -1.600371 -3.664051
C 3.196768 -0.752573 -2.627606
C 5.308127 -4.457154 -1.737122
C 3.960738 -0.494776 1.514538
C 5.266071 -0.007703 1.716221
C 6.002293 -0.455791 2.821393
C 5.437742 -1.374837 3.720577
C 4.129500 -1.860547 3.536340
C 3.400497 -1.413380 2.419276
C 3.493030 -2.814835 4.527021
C -3.136634 1.642086 -1.049037
C -1.955848 2.354246 -1.322930
C -1.983964 3.571476 -2.024120
C -3.231302 4.071266 -2.447311
C -4.418322 3.378804 -2.165140
C -4.378586 2.166696 -1.459363
C -0.698266 4.322144 -2.312755
H -2.544711 0.801902 2.867698
H -1.312572 1.870813 4.718297
H 1.187893 2.091688 4.604807
H 2.419950 1.208962 2.663743
H 5.291246 1.031975 -1.467418
H 5.962893 3.354952 -2.101068
H 4.541037 5.289964 -1.443736
H 1.769175 2.605050 0.488629
H 2.376020 -1.756765 2.260503
H 6.015422 -1.714830 4.584184
H 7.016523 -0.085458 2.985864
H 5.694627 0.718484 1.024260
H 2.655882 0.162857 -2.854961
H 3.390422 -1.336853 -4.697791
H 4.630051 -3.436672 -4.191376
H 4.387893 -2.576580 0.024727
H -4.641069 -0.117809 -2.616234
H -5.452607 -2.081246 -3.911035
H -4.760352 -4.385993 -3.264890
H -2.446173 -2.768646 -0.000987
H -4.327539 2.325382 1.268823
H -6.055300 2.398650 3.062955
H -7.008520 0.282430 3.972369
H -4.541444 -1.995657 1.271197
H -5.304861 1.643590 -1.216038
H -5.377953 3.786058 -2.491276
H -3.273037 5.015366 -2.997438
H -1.000969 1.956500 -0.974343
H 1.252270 4.924868 0.440107
H 2.712989 5.912208 0.703245
H 1.940746 5.887364 -0.896168
H 5.566136 -4.526657 -0.668912
H 4.683981 -5.331852 -1.991214
H 6.239682 -4.543177 -2.322036
H 4.235721 -3.209448 5.237493
H 2.703658 -2.304278 5.105191
H 3.017771 -3.665512 4.011765
H -6.272703 -3.126065 2.547746
H -5.858640 -2.578428 4.189148

H -7.454987 -2.193036 3.509500
H -2.893403 -5.224085 -0.136064
H -3.825221 -5.901291 -1.504371
H -2.142757 -5.369738 -1.740078
H -0.703732 5.319150 -1.839145
H 0.176852 3.769891 -1.938934
H -0.566036 4.476291 -3.397067
H -0.116593 -2.421033 -2.791163

58-PH(TS)
C -1.764600 3.161628 0.192363
Si -2.670256 1.479613 0.205098
C -4.102298 1.604626 -1.048840
C -3.359636 1.228907 1.959446
C -1.446536 0.083853 -0.368397
C -0.719983 0.463177 -1.716332
C 0.687876 -0.196076 -1.783089
C 1.430123 -0.018440 -0.403267
Si 2.362888 1.693978 -0.331388
C 4.128358 1.589496 -1.054669
Si -2.437733 -1.582507 -0.557775
C -3.787588 -1.797745 0.762741
Si -0.000413 -0.114582 0.833835
P -0.003451 -0.660101 2.896843
C -3.230464 -1.617530 -2.294568
C -1.309953 -3.111257 -0.454490
Si 2.731656 -1.415532 -0.012614
C 3.733038 -1.759013 -1.601859
C 3.824752 -0.935493 1.467936
C 1.961459 -3.092844 0.465041
C 1.527753 3.003361 -1.439437
C 2.429117 2.352552 1.453655
H -0.589946 1.554026 -1.771256
H -1.311083 0.175315 -2.599839
H 1.263514 0.232848 -2.621494
H 0.564523 -1.270196 -2.009761
H -3.607568 2.213250 2.394045
H -4.274934 0.619016 1.967627
H -2.622534 0.737034 2.615420
H -4.729129 2.485968 -0.826654
H -3.731448 1.709770 -2.082401
H -4.752239 0.715997 -1.014154
H -2.417822 3.927398 0.645398
H -0.827742 3.145585 0.775393
H -1.524338 3.500569 -0.827850
H -3.886627 -2.501992 -2.374438
H -3.839258 -0.725560 -2.506622
H -2.468234 -1.703186 -3.087073
H -4.176837 -2.829405 0.701886
H -3.388062 -1.645242 1.777434
H -4.639217 -1.113139 0.623651
H -1.910183 -4.021562 -0.629533
H -0.515590 -3.087942 -1.216896
H -0.830660 -3.220291 0.530610
H 4.578377 2.596479 -0.995019
H 4.800989 0.889638 -0.540518

H 4.098766 1.307612 -2.120443
H 3.119416 3.211659 1.519991
H 1.437281 2.701592 1.790120
H 2.763934 1.586185 2.168630
H 2.209533 3.868246 -1.521364
H 1.350288 2.629747 -2.461479
H 0.574611 3.370751 -1.038006
H 2.792905 -3.764194 0.745655
H 1.297090 -3.019219 1.340099
H 1.413206 -3.578393 -0.355042
H 4.384908 -2.635573 -1.440742
H 3.056798 -2.005154 -2.438650
H 4.368086 -0.919828 -1.918269
H 4.557090 -1.739976 1.657480
H 4.381568 0.005681 1.353625
H 3.179831 -0.849128 2.358848
H 0.088017 0.738346 3.241369

59-PH(TS)
C -5.095531 -1.687599 0.065043
C -4.034353 -0.803053 -0.217877
C -4.179666 0.583327 0.075835
C -5.383873 1.047499 0.643613
C -6.432517 0.156421 0.919757
C -6.288353 -1.211346 0.630773
Si -2.379110 -1.283924 -0.993520
C -2.544230 -1.531006 -2.876034
Si -2.679218 1.642085 -0.373104
C -2.233662 2.900770 0.981342
C -1.320675 0.313353 -0.681696
C -0.303010 0.652244 -1.819350
C 0.998786 -0.159238 -1.601666
C 1.400954 -0.127828 -0.079059
Si -0.247541 -0.041061 0.822262
P -0.845953 -0.493206 2.815996
Si 2.655063 -1.535860 0.364880
C 2.684833 -1.983666 2.206910
C 4.286871 -0.685337 -0.108601
C 4.212463 0.736769 -0.121751
C 5.366398 1.492021 -0.417326
C 6.582285 0.850611 -0.702640
C 6.656864 -0.552824 -0.689941
C 5.516133 -1.315355 -0.391421
Si 2.498734 1.436049 0.292947
C 2.087958 2.932673 -0.808383
C 2.361375 -3.110086 -0.662799
C 2.389775 1.968951 2.114651
C -2.977825 2.577736 -2.008699
C -1.682961 -2.889749 -0.238517
H -0.063215 1.726964 -1.796903
H -0.716357 0.444929 -2.819479
H 0.807957 -1.202414 -1.908172
H -1.576048 -1.778431 -3.343808
H -3.242392 -2.357333 -3.094300
H -2.935704 -0.622786 -3.363311
H -0.713682 -3.163676 -0.688291

H -1.555343 -2.814017 0.854009
H -2.377912 -3.726880 -0.427642
H -2.081840 3.138875 -2.325445
H -3.246520 1.884216 -2.822909
H -3.803693 3.301482 -1.898461
H -1.298212 3.438074 0.742368
H -3.026561 3.660915 1.092105
H -2.105044 2.393345 1.950420
H 1.805309 0.215337 -2.256152
H -5.505258 2.108195 0.883742
H -7.359657 0.523902 1.366447
H -7.103108 -1.904523 0.853847
H -4.992219 -2.756776 -0.144402
H 1.424776 2.455154 2.337814
H 2.486108 1.109342 2.795740
H 3.192470 2.688628 2.352062
H 1.106127 3.369524 -0.559393
H 2.845214 3.721909 -0.656803
H 2.087479 2.673404 -1.878893
H 1.697393 -2.312237 2.566667
H 3.420208 -2.788594 2.384399
H 2.977136 -1.119790 2.824255
H 1.425662 -3.615284 -0.370609
H 2.322466 -2.908473 -1.745205
H 3.185105 -3.823739 -0.486613
H 5.321163 2.585414 -0.435014
H 7.470505 1.441653 -0.939129
H 7.603507 -1.049751 -0.916329
H 5.588341 -2.407328 -0.386224
H -0.654110 0.895097 3.158172

60-PH(TS)
C 2.233286 3.218413 0.553499
C 1.200555 2.654140 -0.227019
C 0.688913 3.400097 -1.307432
C 1.188182 4.679038 -1.596627
C 2.207335 5.232993 -0.807660
C 2.727673 4.497361 0.270247
C 0.673551 1.302694 0.115776
C 1.600341 0.110551 0.158610
C 3.038839 0.280803 -0.181688
C 3.440886 0.875508 -1.397278
C 4.799752 1.005869 -1.714289
C 5.780763 0.557545 -0.815329
C 5.392148 -0.025390 0.402547
C 4.034160 -0.165124 0.714665
C 1.044933 -1.086361 0.550216
C 1.724132 -2.395399 0.557999
C 2.591507 -2.787313 -0.494619
C 3.152874 -4.068465 -0.528232
C 2.867103 -4.996708 0.488765
C 2.008549 -4.625528 1.535761
C 1.438163 -3.344412 1.570906
Si -0.740639 -0.735862 1.157159
P -1.350907 -1.182144 3.204765
C -2.047526 -1.408248 -0.126182

N -1.871041 -2.211906 -1.214387
C -3.060734 -2.351179 -1.930097
C -4.003626 -1.610419 -1.259233
N -3.364741 -1.049367 -0.157091
C -0.596886 -2.851550 -1.572698
C -4.072201 -0.209037 0.823810
C -5.450907 -1.371304 -1.554108
C -3.188903 -3.175041 -3.173674
C -0.611411 1.071526 0.520131
C -1.730012 2.027613 0.567227
C -2.233506 2.474431 1.811563
C -3.374662 3.286619 1.869685
C -4.046105 3.658400 0.692763
C -3.562476 3.213150 -0.549434
C -2.417458 2.404866 -0.608941
H 2.681546 1.242673 -2.089092
H 5.092413 1.465975 -2.660938
H 6.840009 0.666281 -1.059150
H 6.148304 -0.371923 1.110616
H 3.727172 -0.625694 1.654689
H -0.094994 2.968147 -1.928437
H 0.780690 5.240845 -2.440447
H 2.596850 6.228577 -1.032169
H 3.523289 4.918844 0.888745
H 2.646922 2.642343 1.382527
H -1.735047 2.154615 2.727106
H -3.746215 3.624213 2.840021
H -4.936635 4.289114 0.742439
H -4.076203 3.495674 -1.472023
H -2.062832 2.029789 -1.571023
H 2.814349 -2.076094 -1.290842
H 3.814748 -4.345300 -1.352775
H 3.307513 -5.996169 0.462147
H 1.778192 -5.336784 2.332904
H 0.763004 -3.058094 2.381270
H -5.730591 -1.863486 -2.495790
H -6.099886 -1.766894 -0.754440
H -5.664550 -0.293581 -1.648895
H -2.968505 -4.239437 -2.985316
H -4.216659 -3.106849 -3.556095
H -2.507396 -2.827487 -3.968325
H -0.759971 -3.491741 -2.446657
H 0.153343 -2.085921 -1.802078
H -0.234840 -3.454531 -0.732237
H -4.986322 -0.737091 1.130469
H -3.423264 -0.061598 1.696937
H -4.322506 0.758316 0.368260
H -2.442296 -2.004425 2.739468

61-PH(TS)
N -3.156268 -1.061512 0.352021
C -1.790231 -1.127639 0.279594
N -1.388585 -1.678062 1.471976
C -2.493069 -1.965617 2.273223
C -3.607539 -1.589084 1.561666
Si -0.695316 -0.567553 -1.283402

P -1.566926 -1.141075 -3.192653
C 0.031853 -1.769428 1.907262
C 0.411828 -3.138090 2.492779
C -2.424821 -2.584238 3.637633
C -5.045770 -1.781216 1.941681
C -4.021845 -0.381225 -0.664403
C -4.611964 0.919192 -0.100938
C -0.357867 1.252890 -0.782773
C -1.377530 2.313453 -0.729749
C -1.573507 3.112804 0.422998
C -2.557825 4.108597 0.447122
C -3.364397 4.335686 -0.682188
C -3.187105 3.544166 -1.828125
C -2.214758 2.534126 -1.850508
C 0.951665 1.371125 -0.381792
C 1.536226 2.647592 0.115954
C 2.192609 2.713967 1.364107
C 2.704369 3.928506 1.840499
C 2.581105 5.096860 1.071536
C 1.938792 5.040714 -0.176626
C 1.419307 3.828324 -0.648027
C 1.788461 0.125903 -0.471290
C 1.139231 -1.010605 -0.899414
C 1.731960 -2.327034 -1.180861
C 3.045129 -2.500383 -1.685016
C 3.553275 -3.777490 -1.945463
C 2.768031 -4.920425 -1.712661
C 1.455850 -4.768743 -1.238859
C 0.942408 -3.489321 -0.991956
C 3.219194 0.162164 -0.062566
C 4.122685 1.096612 -0.610512
C 5.465627 1.112186 -0.208844
C 5.925444 0.204467 0.758590
C 5.033267 -0.726270 1.317096
C 3.695059 -0.748183 0.905467
C 0.379346 -0.579091 2.814713
C -5.069686 -1.334765 -1.253392
H 2.308658 1.805073 1.955722
H 3.206701 3.960429 2.810206
H 2.985759 6.042330 1.439629
H 1.841254 5.943265 -0.784192
H 0.909118 3.783842 -1.611254
H 3.004990 -1.485155 1.319761
H 5.382281 -1.437680 2.069206
H 6.970506 0.221928 1.075604
H 6.152014 1.839715 -0.647563
H 3.763103 1.814624 -1.348412
H 3.659838 -1.623582 -1.883677
H 4.566938 -3.881968 -2.339497
H 3.169411 -5.915714 -1.916069
H 0.824750 -5.646194 -1.077967
H -0.087629 -3.378788 -0.647133
H -0.936971 2.950247 1.294125
H -2.692450 4.713985 1.346903
H -4.124936 5.119757 -0.665489
H -3.812281 3.708851 -2.709269

H -2.092120 1.898668 -2.729852
H -5.111609 -2.071092 2.999196
H -5.645371 -0.872179 1.805181
H -5.513825 -2.581232 1.345890
H -1.699703 -2.067953 4.283325
H -3.408704 -2.520852 4.121588
H -2.135266 -3.646367 3.595820
H 0.601452 -1.647303 0.985809
H -3.333734 -0.122935 -1.481278
H 1.508730 -3.221073 2.461557
H 0.093141 -3.264501 3.536340
H 0.000579 -3.954476 1.881942
H 1.455747 -0.607566 3.042801
H 0.162730 0.364671 2.293618
H -0.178921 -0.604752 3.763670
H -5.485637 -0.860933 -2.155499
H -4.602954 -2.283249 -1.556557
H -5.898356 -1.535474 -0.559277
H -5.048913 1.482556 -0.937365
H -5.405394 0.743902 0.640845
H -3.826610 1.543707 0.344395
H -2.482861 -2.050563 -2.549078

62-PH(TS)
C 2.235063 0.602037 2.801630
C 1.890215 0.146334 1.518781
C 2.559326 0.694953 0.377261
C 3.555120 1.666211 0.544503
C 3.910392 2.093319 1.839772
C 3.249819 1.566994 2.957060
N 0.867358 -0.743544 1.166564
C -0.004485 -1.335831 2.180074
C 0.472202 -2.677717 2.817602
C -0.697287 -3.191559 3.687164
N 2.038004 0.218051 -0.827649
C 2.806096 0.296021 -2.073888
C 4.135024 -0.557795 -2.160225
C 4.225282 -1.079365 -3.614779
Si 0.554195 -0.748670 -0.609703
P 0.565561 -2.506362 -1.861550
C -1.212939 0.356804 -0.553046
N -1.354206 1.511736 0.189706
C -2.697734 1.843137 0.341558
C -3.428295 0.900838 -0.399466
N -2.501155 -0.005023 -0.910860
C -3.333895 2.872258 1.054560
C -4.724946 2.957133 0.946128
C -5.454214 2.056801 0.133824
C -4.820422 1.016696 -0.553972
C -0.299665 2.444005 0.632500
C 0.005094 3.611135 -0.356349
C 0.480927 3.058558 -1.712185
C -2.924403 -1.107864 -1.798497
C -3.529223 -2.388442 -1.130468
C -2.756706 -2.792315 0.136186
C 0.798281 -3.712753 1.725246

C 1.715840 -2.483057 3.708674
C -5.021106 -2.218996 -0.768680
C -3.405991 -3.505476 -2.195465
C -1.200054 4.545995 -0.588453
C 1.142077 4.422087 0.308174
C 5.391439 0.301409 -1.875254
C 4.130091 -1.758503 -1.192179
H 1.727663 0.202855 3.677303
H 3.517856 1.900516 3.961863
H 4.695217 2.842249 1.963581
H 4.039859 2.095085 -0.331102
H 2.121613 -0.055432 -2.859144
H 3.054136 1.350254 -2.302172
H 5.155669 -1.652940 -3.760215
H 3.366598 -1.732512 -3.837412
H 4.224707 -0.241108 -4.333925
H 6.297249 -0.252023 -2.175423
H 5.366649 1.244905 -2.448578
H 5.482171 0.541860 -0.806861
H 5.081034 -2.308448 -1.294283
H 4.036594 -1.424882 -0.147703
H 3.305583 -2.448070 -1.420076
H -0.975097 -1.529045 1.701414
H -0.187443 -0.601327 2.987012
H 2.028040 -3.454158 4.128301
H 2.555564 -2.067281 3.133482
H 1.501890 -1.804448 4.551695
H -0.416654 -4.131646 4.189231
H -0.965556 -2.454824 4.464456
H -1.590561 -3.384859 3.069596
H 1.080518 -4.671344 2.192434
H -0.061726 -3.884469 1.062458
H 1.632235 -3.370335 1.096247
H -5.383253 0.326848 -1.176344
H -6.535381 2.172036 0.043948
H -5.255380 3.744081 1.484154
H -2.765469 3.586929 1.645343
H -3.664803 -0.676405 -2.490901
H -2.041171 -1.374324 -2.381011
H -0.627886 2.851804 1.600044
H 0.612309 1.878341 0.812504
H -3.158612 -3.741116 0.527550
H -1.687648 -2.925079 -0.083522
H -2.874187 -2.027199 0.920025
H -3.884305 -4.425944 -1.825240
H -3.906701 -3.214665 -3.135097
H -2.348367 -3.720772 -2.408063
H -5.429361 -3.192157 -0.452144
H -5.162302 -1.511086 0.061141
H -5.609021 -1.873839 -1.637023
H -0.891387 5.367677 -1.254608
H -2.043442 4.023523 -1.062917
H -1.552319 4.992839 0.355107
H 0.706345 3.893951 -2.394525
H 1.381681 2.448986 -1.585411
H -0.294268 2.432677 -2.183643

H 1.443834 5.249520 -0.354063
H 0.804305 4.856061 1.264684
H 2.018633 3.787453 0.505113
H -0.663356 -2.288747 -2.549262

63-PH(TS)
C -2.820728 1.242779 0.334100
C -2.260258 0.021094 -0.119794
C -3.075510 -1.037967 -0.590085
C -4.468958 -0.850498 -0.610294
C -5.042305 0.344550 -0.160794
C -4.221104 1.374341 0.312790
N -0.832543 -0.152208 -0.129321
Si 0.188492 0.079415 -1.665088
P -0.362630 1.711106 -2.959247
C -2.483195 -2.361898 -1.067406
C -3.087039 -3.564736 -0.308016
C -1.970332 2.403731 0.847145
C -2.247776 2.677917 2.343863
C -0.147133 -0.298734 1.032077
C 1.236233 -0.270914 1.165505
C 1.536955 -0.613912 2.629043
C 0.311264 0.056619 3.317625
C -0.727868 -0.639351 2.397397
C -0.371391 -2.153942 2.640878
C 1.183621 -2.129018 2.856107
P 2.142538 0.021188 -0.322859
C 3.037555 1.699150 -0.202797
C 1.930779 2.714171 0.184452
C 3.294624 -1.456564 -0.674467
C 4.222894 -1.724177 0.534005
C 2.387652 -2.697032 -0.872103
C 4.135046 -1.237459 -1.951253
C -2.665592 -2.523296 -2.593722
C -2.201969 3.683793 0.013462
C 4.121557 1.695287 0.898412
C 3.661466 2.115918 -1.553496
H 0.210339 -1.339122 -2.151794
H 3.979102 3.169612 -1.477525
H 4.548211 1.516911 -1.800186
H 2.940268 2.040698 -2.380004
H 4.432713 2.737509 1.085013
H 3.742159 1.280228 1.844700
H 5.015152 1.133112 0.591386
H 2.394773 3.713137 0.252020
H 1.127071 2.749622 -0.568186
H 1.489099 2.464944 1.160702
H -4.667748 2.308010 0.660877
H -6.126882 0.473688 -0.180237
H -5.107893 -1.656362 -0.977459
H -0.911570 2.135965 0.738409
H -1.603526 3.497875 2.703373
H -3.297134 2.979699 2.495942
H -2.056033 1.788154 2.962565
H -1.565295 4.498443 0.398758
H -1.945860 3.500257 -1.040292

H -3.252368 4.013511 0.079393
H -1.403666 -2.348768 -0.861536
H -2.213583 -3.469569 -2.935357
H -3.736338 -2.536702 -2.856513
H -2.190296 -1.692112 -3.137555
H -2.607646 -4.500464 -0.640458
H -2.939025 -3.460574 0.779086
H -4.169098 -3.653820 -0.497181
H 4.792473 -2.648100 0.333850
H 4.945520 -0.914323 0.696155
H 3.646048 -1.873961 1.457407
H 4.608538 -2.194600 -2.228939
H 3.515596 -0.906328 -2.799841
H 4.938293 -0.504792 -1.790200
H 3.033319 -3.590651 -0.914061
H 1.677407 -2.817604 -0.040385
H 1.816659 -2.636895 -1.807657
H 2.527580 -0.321968 3.001998
H -1.787005 -0.394388 2.529488
H -0.893543 -2.516636 3.539466
H -0.677691 -2.780636 1.790584
H 1.717212 -2.786976 2.156534
H 1.443858 -2.437062 3.882041
H 0.196511 -0.226918 4.377422
H 0.308472 1.151485 3.216443
H 0.985189 2.206598 -3.015958

64-PH(TS)
C 2.866845 -1.438988 -0.732374
C 2.078868 -0.675357 0.170079
C 2.683812 0.036724 1.242167
C 4.086821 0.049333 1.332268
C 4.879947 -0.651706 0.418510
C 4.267153 -1.409530 -0.584328
N 0.652507 -0.568197 -0.031536
C -0.211781 -1.423077 0.575934
C -1.597131 -1.297802 0.583723
C -2.140594 -2.509751 1.354604
C -1.789848 -2.350883 2.876545
C -0.225239 -2.400671 2.872250
C 0.131022 -2.676984 1.366697
C -1.073097 -3.572170 0.947979
P -2.260608 0.143728 -0.193482
C -3.639337 -0.325409 -1.421213
C -3.201849 -1.626713 -2.138961
C 1.880653 0.718675 2.348033
C 2.250927 0.106241 3.723692
C 2.262357 -2.330731 -1.815008
C 2.432241 -3.824017 -1.443243
Si -0.151741 0.608818 -1.258447
P 0.011048 0.060371 -3.349393
C 0.687261 2.264731 -0.851453
C 0.047160 3.473844 -0.505138
C 0.766630 4.670197 -0.352601
C 2.153358 4.687814 -0.559950
C 2.808826 3.503909 -0.937638

C 2.086562 2.313398 -1.086418
C -2.941081 1.324841 1.164005
C -3.957768 0.618938 2.098114
C -1.712168 1.710142 2.023919
C -3.601588 2.581498 0.554955
C 2.092111 2.247937 2.410444
C 2.886871 -2.066335 -3.202790
C -4.974365 -0.616663 -0.695197
C -3.875658 0.823956 -2.431140
H -4.586982 0.473301 -3.197920
H -4.316486 1.702626 -1.938982
H -2.952402 1.135407 -2.937279
H -5.668246 -1.055190 -1.432357
H -4.854387 -1.335514 0.128874
H -5.439247 0.300260 -0.308005
H -3.960580 -1.860809 -2.905729
H -2.222126 -1.531446 -2.624387
H -3.156412 -2.463027 -1.425049
H 4.880721 -1.991253 -1.274554
H 5.969036 -0.625575 0.500815
H 4.557322 0.612727 2.140604
H 1.189343 -2.111903 -1.893821
H 1.991709 -4.457450 -2.231057
H 3.499980 -4.084299 -1.350182
H 1.938220 -4.067463 -0.490011
H 2.348547 -2.651093 -3.964810
H 2.809749 -1.004877 -3.477531
H 3.948614 -2.365442 -3.225356
H 0.816475 0.530222 2.159087
H 1.540549 2.662401 3.271540
H 3.160682 2.480736 2.549560
H 1.747658 2.747523 1.499124
H 1.550925 0.461885 4.498175
H 2.230066 -0.993536 3.703621
H 3.266356 0.415213 4.020464
H -4.033109 1.203103 3.031621
H -4.961605 0.562528 1.662372
H -3.635917 -0.396076 2.362084
H -3.761562 3.324813 1.354511
H -2.989722 3.051207 -0.228425
H -4.583333 2.343682 0.119171
H -2.042221 2.405958 2.814009
H -1.289034 0.817243 2.507080
H -0.918708 2.198715 1.445659
H -3.189063 -2.770953 1.155273
H 1.143983 -3.060170 1.205958
H 0.156800 -3.220307 3.499816
H 0.215469 -1.463445 3.227746
H -2.164593 -1.413723 3.307461
H -2.214618 -3.187000 3.455708
H -1.133974 -4.502857 1.537768
H -1.084780 -3.801190 -0.127507
H 2.625252 1.414344 -1.390585
H 3.887345 3.504346 -1.111424
H 2.716797 5.615856 -0.440084
H 0.240548 5.587242 -0.075901

H -1.031601 3.494874 -0.351477
H -1.388755 0.148478 -3.612320

65-PH(TS)

C	0.717128	-0.935208	3.249179
C	-0.536405	-0.065854	2.930658
C	-0.402764	0.049581	1.412280
C	0.971826	0.067876	1.133121
C	1.695495	-0.013021	2.468697
C	1.433158	1.368311	3.178584
C	-0.091592	1.303590	3.550404
N	1.530209	0.187367	-0.090912
Si	0.308840	0.365450	-1.488805
P	-1.441595	0.104827	0.023451
N	-2.599100	-1.148793	-0.126494
C	-2.447524	-2.626312	-0.086705
C	-3.258035	-3.166853	1.112592
C	2.947075	0.021888	-0.279678
C	3.734877	1.169296	-0.543072
C	5.110898	0.994617	-0.773784
C	5.694998	-0.276549	-0.727236
C	4.903099	-1.395103	-0.443952
C	3.519509	-1.274641	-0.219857
C	3.135201	2.573308	-0.575197
C	3.160897	3.148064	-2.009328
C	2.701356	-2.527375	0.085070
C	2.760035	-3.536781	-1.082964
P	0.483376	-0.980282	-3.156069
C	3.169790	-3.194073	1.399971
C	3.851651	3.519621	0.414458
N	-2.781670	1.193338	0.030828
Si	-3.994060	-0.070876	-0.271247
C	-4.810107	-0.023549	-1.976419
C	-2.778202	2.647118	-0.266195
C	-4.126924	3.211581	0.230264
C	-1.630407	3.343155	0.493907
C	-2.639475	2.905142	-1.784536
C	-5.308245	-0.230009	1.079359
C	-2.999073	-3.205765	-1.407299
C	-0.970800	-3.037994	0.067476
H	0.329706	1.869204	-1.577592
H	5.357938	-2.386963	-0.402700
H	6.765756	-0.394870	-0.908273
H	5.729157	1.869514	-0.985473
H	1.651238	-2.237533	0.207521
H	2.543027	-4.074666	1.618942
H	4.214996	-3.534137	1.315526
H	3.104866	-2.501115	2.252978
H	2.162815	-4.429986	-0.833335
H	2.349612	-3.084761	-1.997760
H	3.797124	-3.860851	-1.271634
H	2.083295	2.505447	-0.264441
H	2.704646	4.151959	-2.026798
H	4.197540	3.232508	-2.375213
H	2.604024	2.498807	-2.702609
H	3.372240	4.512481	0.401715

H	3.809821	3.122148	1.441476
H	4.911667	3.651886	0.143740
H	-1.503581	-0.440506	3.292204
H	2.749817	-0.302282	2.410091
H	2.064387	1.442801	4.077241
H	1.676764	2.213474	2.518342
H	-0.663003	2.143856	3.134852
H	-0.229359	1.295811	4.643864
H	0.952718	-0.986995	4.325531
H	0.657537	-1.949251	2.827794
H	-4.167795	4.297309	0.050893
H	-4.969317	2.749483	-0.311997
H	-4.251325	3.021451	1.307390
H	-1.658677	4.425469	0.291375
H	-1.736291	3.180520	1.576639
H	-0.651154	2.958749	0.171288
H	-2.657824	3.987898	-1.992085
H	-1.690424	2.498658	-2.161961
H	-3.468180	2.431248	-2.331960
H	-3.172320	-4.264196	1.168016
H	-2.878883	-2.733067	2.051465
H	-4.324952	-2.909469	1.014579
H	-2.939685	-4.306193	-1.395671
H	-4.054912	-2.919253	-1.547348
H	-2.411927	-2.824057	-2.255930
H	-0.905003	-4.137252	0.052620
H	-0.364089	-2.640762	-0.762136
H	-0.559893	-2.674225	1.020104
H	-5.958352	-1.106183	0.914068
H	-4.839069	-0.333538	2.070341
H	-5.957884	0.661923	1.098211
H	-5.453148	-0.906045	-2.136702
H	-5.447288	0.870168	-2.093336
H	-4.048286	-0.009080	-2.771616
H	-0.952411	-1.145516	-3.134995

66-PH(TS)

C	1.460624	-3.214636	1.963513
C	0.173774	-2.425206	2.328441
C	0.156083	-1.382561	1.200545
C	1.493015	-1.099814	0.900654
C	2.336796	-1.940651	1.864817
C	2.129290	-1.317435	3.292067
C	0.652199	-1.713209	3.641456
N	2.018195	-0.260814	-0.024175
C	3.464672	-0.163958	-0.135750
C	4.181317	-1.158925	-0.843888
C	5.567438	-0.991920	-1.004302
C	6.230656	0.118732	-0.470109
C	5.512394	1.065368	0.266816
C	4.124911	0.937624	0.461237
C	3.499108	-2.388007	-1.436986
C	3.401957	-2.268299	-2.973688
C	3.391636	1.975257	1.309049
C	3.307526	3.337062	0.582590
P	-1.257225	-0.802175	0.365747

N	-2.034297	-1.917980	-0.668070
C	-1.456272	-2.868583	-1.649916
C	-2.511863	-3.086431	-2.754077
Si	1.060093	0.932626	-1.070969
P	1.723598	1.428605	-3.040577
C	0.005359	1.798835	0.241098
C	-0.817396	0.683101	-0.536132
C	-1.964014	1.130921	-1.412845
C	-2.009553	0.860224	-2.793810
C	-3.115017	1.248386	-3.566009
C	-4.188243	1.934063	-2.974893
C	-4.139188	2.242915	-1.606223
C	-3.036560	1.843969	-0.837812
C	-0.385753	3.235783	0.238400
C	-0.675098	3.947051	-0.948495
C	-0.992609	5.309929	-0.903539
C	-1.017727	5.999555	0.320891
C	-0.718209	5.309337	1.505343
C	-0.410692	3.941310	1.461897
C	4.199990	-3.701342	-1.023035
C	4.045262	2.141584	2.700074
N	-2.698278	-0.798518	1.287500
Si	-3.556647	-1.943268	0.234753
C	-5.040532	-1.275962	-0.714783
C	-3.073534	-0.093117	2.534830
C	-4.493053	0.491021	2.361494
C	-3.081376	-1.109794	3.700843
C	-2.084011	1.045436	2.850302
C	-3.999360	-3.579598	1.080864
C	-0.167473	-2.311092	-2.278788
C	-1.135348	-4.207269	-0.945557
H	6.129746	-1.742060	-1.563528
H	7.306396	0.238156	-0.617275
H	6.030974	1.920170	0.705159
H	2.478711	-2.439474	-1.041275
H	3.634149	-4.563687	-1.412973
H	5.221803	-3.759029	-1.430869
H	4.263051	-3.792313	0.073521
H	2.860493	-3.134484	-3.390518
H	2.881054	-1.341658	-3.258024
H	4.410367	-2.243560	-3.419149
H	2.367245	1.620281	1.473194
H	2.710354	4.049380	1.173774
H	4.317890	3.755387	0.439758
H	2.838834	3.230300	-0.406704
H	3.445781	2.834374	3.313590
H	4.117895	1.176442	3.226768
H	5.060857	2.560663	2.616292
H	-0.752958	-3.004226	2.435606
H	3.383981	-2.062750	1.573362
H	2.845004	-1.763927	3.998951
H	2.290026	-0.230252	3.283654
H	0.033327	-0.844051	3.896176
H	0.620969	-2.414484	4.491199
H	1.795376	-3.901422	2.758933
H	1.385932	-3.754537	1.008492

H	-4.792720	1.032212	3.273022
H	-4.528233	1.177827	1.504348
H	-5.225027	-0.315750	2.190425
H	-3.387035	-0.618004	4.639141
H	-3.789528	-1.926487	3.490069
H	-2.081724	-1.544694	3.837987
H	-2.363240	1.516102	3.805409
H	-1.060042	0.655952	2.942598
H	-2.085701	1.815295	2.068757
H	-2.117759	-3.770384	-3.522416
H	-3.428786	-3.537894	-2.337742
H	-2.771884	-2.124782	-3.220601
H	0.271738	-3.068932	-2.944629
H	-0.363051	-1.404845	-2.861267
H	0.568284	-2.071645	-1.502560
H	-0.694940	-4.924143	-1.657660
H	-0.420303	-4.034456	-0.128058
H	-2.047860	-4.653335	-0.522196
H	-4.318698	-4.341128	0.348625
H	-3.142924	-3.982087	1.644053
H	-4.837069	-3.438955	1.786215
H	-5.364481	-2.001589	-1.480627
H	-5.902100	-1.089869	-0.051361
H	-4.778370	-0.334124	-1.218671
H	-1.147139	0.403580	-3.273831
H	-3.125917	1.031356	-4.636546
H	-5.045246	2.241717	-3.578406
H	-4.954517	2.797757	-1.136203
H	-2.992174	2.108503	0.216274
H	-0.176758	3.406594	2.386496
H	-0.725565	5.832636	2.464759
H	-1.260608	7.064135	0.349451
H	-1.211888	5.839555	-1.833623
H	-0.629139	3.425187	-1.904844
H	0.263763	1.459603	1.252183
H	2.019432	2.777653	-2.633476

67-PH(TS)

C -2.257192 2.117148 2.511894
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C -3.033294 2.954133 0.327430
C -2.988169 4.262634 0.839019
C -2.564570 4.517448 2.147843
C -2.224021 3.446194 2.976226
N -2.587140 0.534888 0.622686
C -3.770498 -0.126654 0.445525
C -3.956584 -1.271917 -0.314986
C -5.416877 -1.700055 -0.100012
C -6.362013 -0.667291 -0.808687
C -6.155666 0.630929 0.045626
C -5.105484 0.190821 1.123279
C -5.594567 -1.267089 1.386715
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C -2.527017 -3.883954 -0.626193
C -3.045494 -4.066639 0.820561
C -3.502621 2.737442 -1.110502

C -4.682497 3.647873 -1.518164
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C -3.157377 0.940364 4.548937
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P -0.271992 -1.900674 1.779134
Si 1.080475 0.458758 0.620698
P 2.155174 2.022526 -1.091797
C 2.089807 2.040746 -3.019896
C 0.763798 2.617181 -3.547674
C 3.762643 1.418791 -0.662098
C 3.807107 0.237900 0.058107
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C 5.996478 -0.426894 -1.006390
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C 5.804916 1.397702 0.525545
N 2.726607 -0.503384 0.466065
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C 3.093448 -1.999877 2.416345
C 3.449704 -3.274835 2.891634
C 3.715226 -4.332357 2.014994
C 3.642979 -4.123162 0.634056
C 3.308811 -2.861869 0.109496
C 2.839114 -0.864422 3.407561
C 2.148012 -1.330604 4.706787
C 3.225634 -2.654360 -1.402808
C 4.228926 -3.509933 -2.206012
C 1.947198 3.776066 -0.352307
C 2.634069 3.770330 1.033377
C 2.576096 4.889963 -1.214594
C 0.442642 4.058472 -0.159812
C 1.795102 -2.924632 -1.905360
C 4.147654 -0.114682 3.749190
C -2.520574 -1.728237 -2.929130
C -3.894267 -2.045081 -3.559920
C -2.254607 -0.218008 -3.104817
C -1.401590 -2.518168 -3.635291
C -2.327658 2.927972 -2.084191
C -0.647484 1.145117 4.222794
C -3.471138 -4.658186 -1.575812
C -1.102274 -4.467924 -0.741134
C 3.276448 2.791576 -3.665897
C 2.174594 0.544205 -3.407942
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H -1.944248 3.631882 4.015045
H -2.525674 5.542241 2.524503
H -3.287404 5.094776 0.199944
H -2.008259 0.041077 2.974008

H -2.986939 0.109938 5.254053
H -3.213282 1.878299 5.126303
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H 0.168471 1.194592 3.484411
H -0.617839 2.058503 4.840592
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H -1.575889 -3.603173 -3.611029
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H -3.028899 0.373641 -2.599495
H -1.275048 0.073989 -2.697156
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H -6.095405 -0.515049 -1.863703
H -7.409142 -1.009188 -0.767714
H -6.640273 -1.304973 1.739967
H -4.940088 -1.823574 2.072734
H 3.858790 -4.948454 -0.046462
H 3.981597 -5.316373 2.408055
H 3.511930 -3.445102 3.967328
H 2.161702 -0.145196 2.926013
H 1.834742 -0.449615 5.288766
H 1.259486 -1.940150 4.485912
H 2.830533 -1.921435 5.340543
H 3.944751 0.686282 4.480320
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H 4.593187 0.341420 2.855228
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H 4.232762 -3.184272 -3.259075
H 5.251302 -3.421812 -1.806671
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H 3.130045 0.104621 -3.083504
H 1.357581 -0.035224 -2.948893
H 3.297442 2.553473 -4.745034
H 3.180882 3.880146 -3.566929
H 4.237029 2.485390 -3.233054
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H 3.716605 3.598431 0.945533

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H 2.501152 5.845294 -0.665209
H 3.639843 4.698412 -1.422800
H 2.045323 5.012942 -2.170113
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H 1.519911 -3.975526 -1.728150
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H 5.465689 -0.774875 1.151244
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H 5.508136 -1.257140 -1.525623
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H 6.906767 1.451646 0.576955
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68-PH(TS)
C 3.216883 1.253533 -0.345390
C 2.670025 -0.000225 0.011521
C 3.380543 -1.208209 -0.169477
C 4.661431 -1.139120 -0.745261
C 5.220248 0.088803 -1.118454
C 4.501115 1.272876 -0.916901
N 1.353906 -0.040188 0.619426
C 1.301948 0.040516 2.050256
C -0.023561 0.002283 2.657598
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C -2.518724 -0.068461 2.822874
C 2.804324 -2.563201 0.231410
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C 2.460645 2.563274 -0.141101
C 3.227063 3.506493 0.813348
N -1.350020 -0.112140 0.615802
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P 0.026699 -0.135394 -2.572133
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C -3.373262 -1.185455 -0.326948
C -4.651963 -1.044649 -0.896248
C -5.217631 0.218224 -1.100974
C -4.508519 1.368792 -0.733465
C -3.229018 1.278156 -0.159721
C -2.787589 -2.581102 -0.132698
C -3.663507 -3.437870 0.810191
C -2.454553 2.545855 0.198301
C -3.305652 3.555486 0.999017
C -1.890408 3.201618 -1.084817
C -2.601095 -3.290499 -1.494212
C 2.641170 -3.481276 -1.001840
C 2.174294 3.249945 -1.496155
C 2.424579 0.149374 2.813243
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H 6.216480 0.123201 -1.565121
H 4.936320 2.230765 -1.208745

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H 4.694953 -3.419787 0.943698
H 3.736241 -2.599235 2.211029
H 2.181971 -4.439044 -0.704956
H 2.008394 -3.004399 -1.766678
H 3.620643 -3.698935 -1.457890
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H 2.659127 4.440111 0.960571
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H 3.115966 3.536205 -1.992451
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H -1.797028 -2.480576 0.335122
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H -3.576585 -3.459871 -1.978831
H -1.984204 -2.679545 -2.170045
H -3.206274 -4.430546 0.953214
H -3.777534 -2.962022 1.797379
H -4.669256 -3.583384 0.383863
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H -3.129778 -0.951872 2.577237
H -0.033541 0.033077 3.747005
H 2.321520 0.208398 3.896592
H 3.424415 0.183290 2.387993
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69-PH(TS)
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N 0.298794 2.653783 0.864348
C 0.551508 3.989703 0.575730
C 0.502978 4.101847 -0.790760
Si -0.005102 -0.104644 -0.395539
P -0.085047 -0.850136 -2.416492
C 0.283366 2.112988 2.226956
C 0.820355 5.026993 1.621030
C 0.686717 5.294008 -1.674605
C 0.090453 2.602067 -2.730272
N 1.318086 -0.650844 0.665438
C 1.189253 -0.951669 2.049295
C 2.281637 -1.141318 2.850577
C 2.550826 -1.076159 0.042688
C 2.729354 -2.457188 -0.242766

C 3.930553 -2.863583 -0.847636
C 4.936734 -1.942291 -1.165278
C 4.753110 -0.589970 -0.863413
C 3.569265 -0.138944 -0.249803
C 1.683692 -3.509437 0.120051
C 1.272987 -4.363937 -1.097624
C 3.431811 1.338302 0.096915
C 4.498765 1.782844 1.122352
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C -2.262623 -3.071449 -0.414404
C -2.626798 -3.968675 0.792068
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71-PH(TS)
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C -5.145033 1.131787 -0.979012
C -4.933631 -0.248765 -0.925095
N -1.437752 -0.379780 0.463779
Si -0.025650 -0.667175 -0.710334
P 0.332491 -2.633760 -1.482667
C -1.841730 2.506946 0.385373
C -1.509225 3.538239 -0.713414
C -3.569756 -2.306041 -0.395535
C -3.655647 -2.916869 -1.814603
N 1.365874 -0.122417 0.441833
C 1.224291 -0.136110 1.776557
C 2.361161 0.286969 2.687370
C 2.662151 0.153264 -0.157851
C 3.651659 -0.867964 -0.170124
C 4.911778 -0.550065 -0.710032
C 5.188324 0.717428 -1.231028
C 4.192753 1.698910 -1.223945
C 2.915760 1.439950 -0.694173
C 3.431303 -2.273803 0.390005
C 3.764592 -3.354387 -0.665311
C 1.883323 2.563553 -0.663493
C 1.714357 3.223430 -2.049227
C -0.003205 -0.445623 2.411206
C -1.266800 -0.466476 1.806605
C -2.493279 -0.514791 2.693680
C 2.257317 3.614234 0.407444
C 4.285799 -2.518888 1.657717

C -2.283149 3.223984 1.682441
C -4.644347 -2.952617 0.511479
H 5.684905 -1.320109 -0.719123
H 6.175228 0.938900 -1.643224
H 4.407195 2.690272 -1.626090
H 2.369180 -2.392068 0.644302
H 4.116552 -3.544262 2.024989
H 5.358887 -2.412954 1.426510
H 4.042346 -1.818714 2.470318
H 3.492675 -4.345431 -0.269106
H 3.197618 -3.190320 -1.591304
H 4.842639 -3.361691 -0.898359
H 0.913670 2.135875 -0.385128
H 1.493892 4.409110 0.447290
H 2.333371 3.153004 1.405279
H 3.228551 4.080098 0.173289
H 0.943722 4.006768 -2.001085
H 2.651493 3.692391 -2.388389
H 1.410653 2.476922 -2.799029
H -4.298239 3.081704 -0.591347
H -6.094536 1.528591 -1.344885
H -5.721087 -0.931857 -1.248299
H -2.579972 -2.541863 0.020784
H -3.489817 -4.005149 -1.766401
H -4.652406 -2.737901 -2.250982
H -2.896400 -2.481010 -2.480011
H -4.470888 -4.038652 0.579108
H -4.633827 -2.534626 1.530548
H -5.652947 -2.794661 0.095885
H -0.921555 1.953420 0.612006
H -1.504026 3.933937 2.006167
H -3.215863 3.787659 1.517687
H -2.456077 2.506387 2.499359
H -0.701639 4.204271 -0.371058
H -1.179674 3.034181 -1.633091
H -2.385944 4.161472 -0.952144
H -2.206344 -0.586886 3.751157
H -3.116509 0.380239 2.550149
H -3.115535 -1.381836 2.426401
H 0.021030 -0.515679 3.497131
H 2.366535 -0.335953 3.593748
H 2.188966 1.330385 3.002267
H 3.341292 0.235605 2.203701
H -0.152063 0.573123 -1.544965
H -1.056624 -2.958767 -1.367965

72-PH(TS)
C 3.746744 -0.733967 -0.376773
C 2.697521 0.144420 -0.017570
C 2.859749 1.553375 -0.101348
C 4.081984 2.062790 -0.571485
C 5.121518 1.207668 -0.955571
C 4.948071 -0.174795 -0.854439
N 1.433646 -0.362467 0.490300
C 1.271855 -0.445888 1.834847
C 2.497504 -0.493239 2.724115

C 1.768172 2.519746 0.353779
C 2.084013 3.101190 1.751850
C 3.647043 -2.250270 -0.251312
C 4.758286 -2.823202 0.661157
C 0.007722 -0.444985 2.438010
C -1.220359 -0.166109 1.793760
C -2.388920 0.243576 2.667350
N -1.359224 -0.185267 0.455155
Si 0.034265 -0.811306 -0.670311
P -0.235237 -2.871763 -1.200967
C -2.675257 0.129766 -0.092789
C -2.961098 1.452002 -0.515761
C -4.268759 1.755777 -0.934568
C -5.272620 0.783297 -0.945398
C -4.966433 -0.520697 -0.547991
C -3.674260 -0.880873 -0.120529
C -1.920664 2.566186 -0.523293
C -2.241617 3.654129 0.526306
C -3.426464 -2.337895 0.267998
C -4.307119 -2.796455 1.454897
N 0.109274 0.381155 -1.924537
C -3.693543 -3.259803 -0.946611
C -1.788693 3.189612 -1.930888
C 1.536025 3.667681 -0.652079
C 3.725073 -2.916824 -1.644761
H 2.211135 -0.482998 3.784218
H 5.759468 -0.845888 -1.141797
H 6.063538 1.619042 -1.324625
H 4.220421 3.143646 -0.633619
H 2.673919 -2.499271 0.195091
H 4.609923 -3.907142 0.791938
H 5.753344 -2.669263 0.212860
H 4.763229 -2.348694 1.655190
H 3.607505 -4.008169 -1.548057
H 2.929791 -2.543566 -2.306056
H 4.702417 -2.713286 -2.113586
H 0.833708 1.954190 0.449436
H 1.297528 3.813238 2.052650
H 2.136122 2.306845 2.510501
H 3.048980 3.633703 1.738792
H 0.660704 4.260258 -0.346324
H 2.403974 4.344765 -0.691294
H 1.360279 3.289167 -1.671073
H -4.496767 2.775356 -1.251113
H -6.284301 1.038505 -1.268635
H -5.740752 -1.289636 -0.568062
H -2.370831 -2.463538 0.545152
H -3.400395 -4.291236 -0.697335
H -4.764367 -3.253116 -1.212487
H -3.107019 -2.942955 -1.819924
H -4.117205 -3.862560 1.659126
H -4.099568 -2.235471 2.379355
H -5.378206 -2.681537 1.220211
H -0.954680 2.124767 -0.263073
H -1.479393 4.450512 0.495481
H -3.223441 4.112711 0.325856

H -2.261745 3.237270 1.545856
H -1.005703 3.963949 -1.932088
H -1.528371 2.412190 -2.663661
H -2.732516 3.663389 -2.243855
H -2.129501 0.147030 3.730061
H -2.656678 1.291929 2.459591
H -3.285960 -0.350165 2.453310
H -0.016973 -0.509940 3.523677
H 3.064335 -1.413366 2.514322
H 3.173699 0.350143 2.524046
H 0.240690 0.032444 -2.868794
H 0.438660 1.335413 -1.808800
H 1.171148 -3.105160 -1.085430

73-PH(TS)
C -2.973928 1.487450 0.148739
C -2.756596 0.113924 -0.133406
C -3.801867 -0.834861 0.031541
C -5.057746 -0.372709 0.468833
C -5.293113 0.978658 0.730348
C -4.251202 1.896183 0.571787
N -1.473685 -0.301569 -0.694293
C -1.383695 -0.387608 -2.041852
C -2.611780 -0.120138 -2.888893
C -3.644881 -2.334781 -0.213751
C -4.650560 -2.890648 -1.251531
C -1.890794 2.548358 -0.012999
C -2.152173 3.446698 -1.242939
C -0.175412 -0.643807 -2.720126
C 1.116978 -0.541853 -2.175991
C 2.300571 -0.591642 -3.119519
N 1.321412 -0.397129 -0.851506
Si -0.027987 -0.841995 0.401268
P 0.085235 -2.902547 0.988256
C 2.619664 0.063623 -0.389503
C 3.622851 -0.858916 -0.005970
C 4.858297 -0.348069 0.438607
C 5.108059 1.025033 0.490189
C 4.113061 1.920704 0.083068
C 2.860027 1.463074 -0.358241
C 3.444420 -2.371759 -0.066457
C 4.472596 -3.020973 -1.023610
C 1.823735 2.478539 -0.834696
C 2.198416 3.050418 -2.222594
N 0.140947 0.406601 1.588661
C 0.514100 0.184327 2.998771
C -0.370515 1.027074 3.936042
C 2.009472 0.481365 3.227288
C 1.631318 3.634853 0.169534
C 3.578239 -2.997034 1.341617
C -3.839453 -3.100178 1.120024
C -1.750974 3.402332 1.266317
H -2.383111 -0.252592 -3.954604
H -5.862983 -1.097097 0.601667
H -6.279206 1.314311 1.058731
H -4.427187 2.954055 0.773299

H -2.628291 -2.530735 -0.581243
H -4.487137 -3.973648 -1.372022
H -5.688742 -2.741844 -0.913294
H -4.548299 -2.422233 -2.242291
H -3.622230 -4.170588 0.975352
H -3.171498 -2.714007 1.903283
H -4.881148 -3.000862 1.468089
H -0.941357 2.032970 -0.180434
H -1.363279 4.212561 -1.330253
H -2.162757 2.859098 -2.174270
H -3.122101 3.961806 -1.149355
H -0.919366 4.114381 1.161367
H -2.665693 3.985339 1.457655
H -1.562623 2.758873 2.136299
H 4.310539 2.993902 0.104596
H 6.073997 1.397312 0.838314
H 5.633636 -1.053143 0.743407
H 2.434809 -2.598907 -0.435145
H 3.380911 -4.078675 1.287109
H 4.596245 -2.844681 1.739093
H 2.851950 -2.558820 2.040270
H 4.276646 -4.102510 -1.099750
H 4.428624 -2.586636 -2.035185
H 5.500087 -2.886176 -0.646963
H 0.864102 1.960362 -0.950345
H 1.447701 3.791986 -2.542825
H 3.181340 3.547356 -2.181538
H 2.244366 2.257609 -2.983422
H 0.820588 4.295558 -0.173486
H 1.380186 3.264650 1.175444
H 2.545573 4.242950 0.254616
H 1.971359 -0.530311 -4.165506
H 3.020176 0.212478 -2.914749
H 2.834866 -1.543681 -2.970567
H -0.242071 -0.773769 -3.798089
H -3.440904 -0.780824 -2.608458
H -2.968425 0.908378 -2.723628
H 0.368258 1.353133 1.289726
H 0.329654 -0.882934 3.198268
H -0.145065 0.800916 4.991614
H -0.187782 2.104667 3.776410
H -1.435333 0.821948 3.746166
H 2.288142 0.310111 4.280939
H 2.635024 -0.154925 2.584339
H 2.233479 1.534719 2.981950
H -1.325791 -3.066860 0.894017

74-PH(TS)
C -2.145694 1.905139 -1.942091
C -0.885453 2.435205 -1.596519
C -0.697188 3.835935 -1.604622
C -1.761752 4.687895 -1.918562
C -3.024798 4.163226 -2.243945
C -3.201531 2.770031 -2.257836
N 0.171232 1.604465 -1.177929
N 0.171670 0.270912 -1.616668

Si 0.377514 -1.172747 -0.676069
P 0.411137 -2.992229 -1.820533
N 1.800307 -0.797892 0.456422
C 1.886562 -1.539742 1.589595
C 0.750237 -2.122519 2.169943
C -0.594114 -1.842811 1.825774
N -0.930075 -1.191065 0.691167
C -2.332728 -0.822278 0.494283
C -3.234455 -1.762078 -0.070457
C -4.583774 -1.385437 -0.219991
C -5.043295 -0.138583 0.200543
C -4.145738 0.764702 0.777931
C -2.782324 0.455796 0.931961
C -2.842671 -3.161107 -0.533852
C -3.003722 -3.278409 -2.068431
C -1.842011 1.487368 1.559702
C -2.379539 2.933163 1.466592
C 2.829504 0.179272 0.143801
C 2.765966 1.455635 0.770101
C 3.730459 2.416872 0.415523
C 4.730000 2.137272 -0.523943
C 4.802817 0.862980 -1.090577
C 3.875666 -0.141411 -0.753980
C 1.748316 1.780365 1.863372
C 1.134942 3.187592 1.720172
C 4.076625 -1.539176 -1.323416
C 3.890065 -1.552432 -2.856533
C 3.239958 -1.760501 2.229831
C 5.465781 -2.101784 -0.939490
C 2.395425 1.643682 3.263330
C -1.674106 -2.316400 2.773998
C -3.686615 -4.263346 0.151081
C -1.538525 1.160632 3.043547
H 3.136779 -2.177910 3.240261
H 5.600145 0.623722 -1.796408
H 5.459573 2.904020 -0.793670
H 3.703543 3.398336 0.890224
H 3.321407 -2.200281 -0.880337
H 5.558882 -3.139443 -1.298859
H 6.275793 -1.510006 -1.395778
H 5.614017 -2.093139 0.152420
H 4.017567 -2.576012 -3.243432
H 2.882206 -1.208339 -3.130443
H 4.637222 -0.901649 -3.341383
H 0.933930 1.050528 1.799911
H 1.654415 1.886727 4.042399
H 2.761213 0.623705 3.446749
H 3.245489 2.338612 3.363761
H 0.422058 3.358419 2.539288
H 1.900740 3.976217 1.787392
H 0.594987 3.292438 0.770739
H -4.510937 1.739725 1.095404
H -6.094636 0.133029 0.081131
H -5.276823 -2.098441 -0.669538
H -1.787187 -3.343334 -0.292975
H -2.629289 -4.255161 -2.410366

H -4.067024 -3.186749 -2.349537
H -2.431192 -2.498774 -2.590468
H -3.310778 -5.252793 -0.154577
H -3.648732 -4.202224 1.250410
H -4.745336 -4.196296 -0.148448
H -0.902120 1.447326 0.996161
H -0.976420 1.989676 3.502097
H -2.476869 1.034570 3.609135
H -0.935611 0.250254 3.157454
H -1.586808 3.637137 1.751965
H -2.709312 3.178556 0.448585
H -3.223523 3.086948 2.160607
H -1.235848 -2.646755 3.725109
H -2.413951 -1.528663 2.968309
H -2.211668 -3.160850 2.316710
H 0.909811 -2.744341 3.048638
H 3.810020 -2.471008 1.607165
H 3.827893 -0.834064 2.274576
H 0.130741 0.144424 -2.630619
H 1.093201 2.035826 -1.258999
H 0.285759 4.246739 -1.358290
H -1.600419 5.768412 -1.915176
H -3.853116 4.830041 -2.490451
H -4.175719 2.342949 -2.505948
H -2.291956 0.826656 -1.930157
H 1.839958 -3.030290 -1.819711

75-PH(TS)
C 3.660327 -0.905462 -0.105322
C 2.673632 0.117565 -0.085611
C 2.967372 1.436008 -0.515257
C 4.281482 1.721883 -0.929320
C 5.275578 0.739441 -0.931560
C 4.956900 -0.560979 -0.531226
N 1.358055 -0.180575 0.474780
C 1.223696 -0.138215 1.814489
C 2.397363 0.280585 2.675631
C 1.936402 2.561046 -0.539517
C 2.263545 3.654752 0.502582
C 3.396182 -2.356187 0.298687
C 4.246430 -2.797975 1.514089
C -0.004403 -0.394261 2.464295
C -1.267211 -0.399480 1.856920
C -2.493613 -0.360534 2.743220
N -1.430594 -0.366147 0.510911
Si -0.030748 -0.776267 -0.633566
P 0.236733 -2.783346 -1.330203
C -2.701613 0.124425 -0.003901
C -2.881565 1.529509 -0.088239
C -4.115377 2.017084 -0.551782
C -5.146274 1.146775 -0.922828
C -4.952227 -0.233192 -0.821446
C -3.737745 -0.773024 -0.355459
C -1.803561 2.527477 0.330019
C -2.234671 3.331056 1.579049
C -3.612888 -2.288998 -0.238563

C -4.688023 -2.885264 0.701812
O -0.119023 0.474730 -1.764814
C -3.727274 -2.950440 -1.632815
C -1.448201 3.481028 -0.829226
C 1.832785 3.174727 -1.953815
C 3.687338 -3.301330 -0.892130
H 2.150302 0.175267 3.740394
H 5.724197 -1.337021 -0.545549
H 6.291044 0.984276 -1.250972
H 4.521977 2.737172 -1.249476
H 2.333815 -2.471412 0.552508
H 4.057968 -3.863240 1.724285
H 5.322440 -2.677967 1.306371
H 4.009752 -2.229163 2.426405
H 3.377179 -4.325429 -0.633077
H 3.129781 -2.994295 -1.787518
H 4.764943 -3.311364 -1.128131
H 0.956799 2.140184 -0.297445
H 1.507123 4.455765 0.457663
H 2.272332 3.249627 1.527296
H 3.250640 4.104079 0.305579
H 1.074802 3.971924 -1.963878
H 2.792758 3.612598 -2.271019
H 1.538858 2.402861 -2.678575
H -4.265324 3.096391 -0.619127
H -6.097664 1.543565 -1.283922
H -5.756111 -0.916915 -1.100086
H -2.623616 -2.527528 0.177030
H -3.576773 -4.038771 -1.548227
H -4.727241 -2.771311 -2.061561
H -2.971367 -2.550321 -2.324035
H -4.533818 -3.971776 0.801188
H -4.657460 -2.437900 1.707855
H -5.698688 -2.721378 0.294022
H -0.896072 1.970380 0.592069
H -1.438293 4.038582 1.863392
H -3.150630 3.909130 1.375402
H -2.430856 2.671261 2.438625
H -0.660379 4.180435 -0.507923
H -1.081272 2.907904 -1.690429
H -2.324378 4.074357 -1.136693
H -2.210378 -0.451425 3.800232
H -3.051592 0.576606 2.599999
H -3.177167 -1.178824 2.475856
H 0.016279 -0.422743 3.551452
H 3.300633 -0.298316 2.448723
H 2.646162 1.334119 2.470887
H -0.116744 0.063794 -2.647980
H -1.160843 -3.044171 -1.186627

76-PH(TS)
C 3.839517 0.655930 -0.464726
C 2.842111 0.133425 0.391545
C 2.985813 -1.136547 1.009721
C 4.136591 -1.888565 0.715446
C 5.113829 -1.408939 -0.162918

C 4.962903 -0.146116 -0.739751
N 1.647917 0.910826 0.705034
Si 0.145271 0.904352 -0.345914
O 0.049525 -0.827157 -0.694677
C 1.978785 -1.678137 2.021772
C 1.593672 -3.143656 1.734866
C 3.776277 2.051396 -1.072634
C 3.655086 1.970196 -2.612388
C 1.618422 1.644905 1.848918
C 2.929391 2.047778 2.486450
C 0.416271 2.016647 2.468460
C -0.875108 1.534753 2.149249
C -1.987550 1.797329 3.140219
N -1.138732 0.867584 1.005200
C -2.484522 0.326603 0.796800
C -3.505529 1.173525 0.291879
C -4.803631 0.641273 0.167219
C -5.092804 -0.671853 0.535856
C -4.071277 -1.489303 1.030176
C -2.752441 -1.020389 1.167447
C -3.291463 2.619582 -0.150210
C -3.577467 2.757695 -1.666327
C -1.675885 -1.951777 1.727815
C -1.936310 -3.439682 1.404470
C -1.505520 -1.763150 3.254146
C -4.199185 3.611422 0.617576
P -0.141292 2.422703 -1.797568
C 2.526344 -1.548826 3.463723
C 5.009890 2.898753 -0.678923
H -1.573644 2.107120 4.108829
H -5.592929 1.281345 -0.229804
H -6.107228 -1.063386 0.433733
H -4.302091 -2.517043 1.306778
H -2.242682 2.900300 0.017509
H -3.966930 4.640726 0.300667
H -5.261918 3.421597 0.395405
H -4.074668 3.551163 1.709916
H -3.301647 3.767647 -2.006465
H -3.000982 2.031073 -2.253082
H -4.650305 2.599835 -1.868007
H -0.730392 -1.684753 1.249504
H -0.790195 -2.503886 3.646036
H -1.119716 -0.763544 3.500129
H -2.467657 -1.906047 3.773664
H -1.053662 -4.033129 1.677420
H -2.791575 -3.836859 1.975568
H -2.128783 -3.582897 0.332406
H 4.265730 -2.865621 1.182637
H 5.993818 -2.015064 -0.388076
H 5.730936 0.241013 -1.411320
H 2.887437 2.560638 -0.675299
H 3.543343 2.980889 -3.037641
H 4.563257 1.513924 -3.039897
H 2.787350 1.365737 -2.911300
H 4.898483 3.922887 -1.069920
H 5.136767 2.952557 0.414474

H 5.932976 2.472489 -1.103247
H 1.067523 -1.071872 1.961355
H 1.792567 -1.951823 4.180896
H 3.464544 -2.117182 3.571850
H 2.725889 -0.500505 3.731845
H 0.850879 -3.475220 2.475186
H 1.170709 -3.253397 0.727629
H 2.465397 -3.810778 1.824562
H 2.758415 2.561422 3.441545
H 3.576844 1.175611 2.652271
H 3.471903 2.721436 1.804192
H 0.497531 2.627228 3.365099
H -2.635421 2.600674 2.759884
H -2.620542 0.911206 3.278379
H 1.261125 2.681937 -1.800885
S 0.215430 -1.665722 -2.064451
O 0.437276 -3.064893 -1.681770
O 1.077261 -0.984676 -3.033310
C -1.584098 -1.581101 -2.697809
F -1.988482 -0.310298 -2.826764
F -1.632533 -2.195459 -3.889843
F -2.392454 -2.216627 -1.831046

77-PH(TS)
C 3.731934 -0.766486 -0.324153
C 2.691659 0.129162 0.020579
C 2.876330 1.533730 -0.059140
C 4.106532 2.019155 -0.535509
C 5.128072 1.148925 -0.928994
C 4.936625 -0.230182 -0.816704
N 1.420195 -0.367015 0.531089
C 1.256906 -0.422731 1.878657
C 2.485127 -0.424660 2.763802
C 1.817682 2.535743 0.396976
C 2.248076 3.241645 1.704956
C 3.624061 -2.276700 -0.151840
C 4.772864 -2.840175 0.718641
C -0.007780 -0.434035 2.482951
C -1.239998 -0.180826 1.839821
C -2.437017 0.128051 2.714195
N -1.377709 -0.197490 0.496664
Si 0.013467 -0.958395 -0.539374
P -0.246601 -3.073691 -0.796317
C -2.684035 0.169215 -0.050108
C -2.917238 1.517815 -0.428697
C -4.214888 1.880092 -0.831700
C -5.251386 0.942872 -0.882972
C -4.994752 -0.383014 -0.532255
C -3.719898 -0.800085 -0.103380
C -1.827458 2.586710 -0.383056
C -1.868694 3.377785 0.944974
C -3.533386 -2.273417 0.248319
C -4.537255 -2.769721 1.316659
S 0.108736 0.346678 -2.299616
C -3.691505 -3.136298 -1.027401
C -1.900783 3.545958 -1.591205

C 1.519405 3.585901 -0.693772
C 3.606647 -2.984661 -1.525615
H 2.200461 -0.480364 3.822860
H 5.738495 -0.914384 -1.099606
H 6.072707 1.545131 -1.307746
H 4.262292 3.097579 -0.596162
H 2.680064 -2.497327 0.364434
H 4.608597 -3.914770 0.898316
H 5.746271 -2.726582 0.215063
H 4.837271 -2.328813 1.692705
H 3.497329 -4.072929 -1.390549
H 2.768488 -2.630342 -2.142713
H 4.549839 -2.793652 -2.064044
H 0.889457 1.990983 0.610451
H 1.475206 3.964422 2.014249
H 2.392808 2.522749 2.525593
H 3.193233 3.788930 1.556551
H 0.745632 4.281854 -0.336440
H 2.417564 4.178379 -0.929133
H 1.167079 3.106728 -1.618033
H -4.415143 2.913943 -1.113169
H -6.250927 1.246033 -1.202333
H -5.795060 -1.122837 -0.585482
H -2.515513 -2.428088 0.631581
H -3.467564 -4.189118 -0.796591
H -4.725062 -3.068540 -1.407280
H -3.002346 -2.809707 -1.818521
H -4.313064 -3.819412 1.564553
H -4.497716 -2.182489 2.247625
H -5.571985 -2.726726 0.939322
H -0.858691 2.079463 -0.432090
H -1.108619 4.175838 0.936036
H -2.857476 3.844580 1.086531
H -1.664670 2.725993 1.807709
H -1.018014 4.199861 -1.601657
H -1.929344 2.979192 -2.533267
H -2.790862 4.193493 -1.541374
H -2.131219 0.228903 3.763999
H -2.936866 1.051237 2.389226
H -3.180915 -0.676759 2.632132
H -0.030848 -0.500935 3.568419
H 3.118554 -1.288517 2.510297
H 3.095828 0.474674 2.600540
H 0.073773 -0.701681 -3.151107
H 1.149193 -3.307002 -0.599489

78-PH(TS)
C -3.702887 -0.837664 -0.110486
C -2.678220 0.145353 -0.064694
C -2.929053 1.488720 -0.448767
C -4.232599 1.831054 -0.852466
C -5.256396 0.881118 -0.901090
C -4.982233 -0.439712 -0.542727
N -1.369525 -0.209013 0.489521
Si 0.027791 -0.965371 -0.520464
Cl 0.134581 0.360641 -2.187122

C -1.867903 2.586377 -0.410119
C -1.853989 3.409809 -1.718082
C -3.501707 -2.304937 0.259168
C -3.670535 -3.187876 -1.001424
C -1.230145 -0.171870 1.832470
C -2.421926 0.176425 2.697892
C -0.002144 -0.439011 2.481299
C 1.264660 -0.448115 1.882909
C 2.492792 -0.470289 2.767118
N 1.434053 -0.389191 0.534627
C 2.694475 0.133858 0.023945
C 3.741065 -0.742006 -0.349598
C 4.931172 -0.180511 -0.849409
C 5.101305 1.203192 -0.939754
C 4.074183 2.052744 -0.516062
C 2.857338 1.542411 -0.031563
C 3.653367 -2.255672 -0.198196
C 3.617852 -2.944912 -1.580971
C 1.790774 2.520138 0.456341
C 1.463429 3.584668 -0.611411
C 2.226324 3.207794 1.772260
C 4.821394 -2.815912 0.648036
P -0.225041 -3.063324 -0.829832
C -2.069543 3.515910 0.809500
C -4.486968 -2.790240 1.349473
H 3.108010 0.428051 2.615067
H 5.738231 -0.847827 -1.156371
H 6.034642 1.619030 -1.325359
H 4.213801 3.134132 -0.560370
H 2.721411 -2.493204 0.332536
H 4.675301 -3.895555 0.812519
H 5.786663 -2.679930 0.134600
H 4.889081 -2.318387 1.629191
H 3.525188 -4.036232 -1.458307
H 2.764004 -2.592808 -2.177479
H 4.548136 -2.735053 -2.134526
H 0.872855 1.958025 0.667794
H 1.446065 3.912660 2.103902
H 2.392281 2.476529 2.577914
H 3.160921 3.772891 1.623337
H 0.667045 4.248163 -0.241654
H 2.343778 4.208840 -0.832702
H 1.124927 3.111662 -1.543101
H -4.444446 2.863741 -1.131625
H -6.260122 1.169471 -1.220920
H -5.773059 -1.190027 -0.589890
H -2.478145 -2.447201 0.631565
H -3.430658 -4.234538 -0.758868
H -4.710785 -3.138797 -1.365286
H -2.999342 -2.864496 -1.809220
H -4.266147 -3.841155 1.595446
H -4.420528 -2.201851 2.278205
H -5.529185 -2.738972 0.994707
H -0.887406 2.111075 -0.316622
H -1.324871 4.328536 0.795478
H -3.073519 3.970966 0.789043

H -1.957808 2.969804 1.759197
H -1.020999 4.126720 -1.697465
H -1.728902 2.751081 -2.589376
H -2.785318 3.984584 -1.843559
H -2.120444 0.267778 3.749686
H -2.885033 1.116997 2.367480
H -3.195909 -0.598901 2.610137
H -0.030706 -0.501184 3.566972
H 2.208446 -0.537824 3.825541
H 3.121329 -1.334311 2.500960
H 1.164917 -3.285972 -0.584110

79-PH(TS)
C -2.880828 -1.924598 -0.696832
C -2.064896 -1.386899 0.325978
C -1.805108 -2.112818 1.518256
C -2.350536 -3.402241 1.643083
C -3.119922 -3.969020 0.621971
C -3.383578 -3.228799 -0.531932
N -1.458103 -0.066834 0.187874
C -1.986248 1.003121 0.849684
C -3.452356 1.049545 1.157219
Si -4.363682 2.428040 0.116866
C -6.224579 2.049954 0.248429
C -1.009403 -1.527360 2.681128
C -1.963083 -1.066620 3.809317
C -3.290014 -1.141663 -1.935384
C -4.828454 -1.005025 -2.014880
C -1.187406 2.093512 1.243605
C 0.218735 2.186259 1.190108
C 0.853645 3.348341 1.926223
N 0.975846 1.317248 0.485465
Si 0.114357 0.182661 -0.709602
P 0.068084 0.881408 -2.714819
C 2.435003 1.415873 0.499322
C 3.175967 0.619194 1.414568
C 4.577301 0.735751 1.403325
C 5.233683 1.606484 0.527712
C 4.485589 2.391870 -0.349076
C 3.079502 2.319650 -0.384401
C 2.503775 -0.286268 2.446196
C 2.179346 0.515741 3.729390
C 2.346660 3.241726 -1.355502
C 2.577136 4.729133 -0.994892
O 0.993115 -1.256785 -0.173145
S 1.427534 -2.605870 -0.938270
O 1.730593 -3.604825 0.093352
O 0.546890 -2.909357 -2.069501
C 3.114537 -2.029803 -1.631269
F 3.991854 -1.907277 -0.619369
C 2.812149 2.992305 -2.810163
C 3.337700 -1.536420 2.799025
C -4.008593 4.119802 0.920248
C -3.765148 2.456038 -1.680519
C 0.029288 -2.522242 3.237293
C -2.737953 -1.793301 -3.222536

F 3.551360 -2.961186 -2.493174
F 2.997886 -0.851431 -2.258363
H -3.999542 -3.655763 -1.325094
H -3.518766 -4.979656 0.731588
H -2.161807 -3.972338 2.553527
H -2.875821 -0.130369 -1.847996
H -5.108028 -0.387154 -2.883781
H -5.306884 -1.990316 -2.132424
H -5.236723 -0.535463 -1.106345
H -2.993651 -1.173460 -4.097546
H -1.646167 -1.901834 -3.173948
H -3.182798 -2.792035 -3.365666
H -0.469248 -0.642372 2.322974
H -1.384323 -0.619581 4.634802
H -2.687932 -0.322878 3.446156
H -2.526577 -1.926461 4.207446
H 0.627720 -2.026760 4.016001
H -0.460452 -3.392505 3.701761
H 0.698681 -2.879521 2.443239
H 5.167249 0.132742 2.092307
H 6.323787 1.673325 0.535661
H 4.989127 3.082083 -1.027682
H 1.269630 3.028820 -1.311624
H 2.174865 3.559288 -3.506195
H 3.855405 3.324005 -2.945786
H 2.744253 1.928555 -3.074649
H 1.985795 5.372031 -1.667075
H 2.294673 4.954038 0.044458
H 3.639772 4.996472 -1.117290
H 1.559638 -0.636565 2.021145
H 1.724717 -0.144810 4.485569
H 3.099567 0.946915 4.157381
H 1.475690 1.336205 3.527362
H 2.746139 -2.201109 3.442606
H 3.619177 -2.092023 1.894929
H 4.252396 -1.270770 3.353855
H 0.330014 3.523800 2.876869
H 1.920674 3.192006 2.119098
H 0.746216 4.257056 1.312061
H -1.701574 2.901476 1.759249
H -3.929686 0.076192 0.981110
H -3.613329 1.321530 2.213239
H -4.069309 3.403224 -2.159340
H -2.665756 2.386539 -1.747258
H -4.189427 1.632818 -2.274505
H -6.815580 2.823313 -0.271995
H -6.476633 1.077521 -0.205491
H -6.558094 2.027972 1.300238
H -4.673591 4.888978 0.490416
H -4.179348 4.107417 2.010722
H -2.971746 4.447000 0.739361
H -1.284011 0.441942 -2.829574

80-PH(TS)
C 4.229771 0.924426 -0.938118
C 3.631452 0.410819 0.226222

C 4.432830 0.501357 1.377133
C 5.703818 1.097137 1.393128
C 6.237615 1.619863 0.209048
C 5.492950 1.530277 -0.973492
B 2.152472 -0.333443 0.139078
C 1.091779 0.744033 -0.648267
C -0.354266 0.416687 -0.569537
N -1.299961 1.422440 -0.579142
Si -3.047344 1.223089 -0.398052
P -4.616671 2.516027 -0.915114
F 4.009284 -0.000572 2.562459
F 6.420546 1.165896 2.533881
F 7.455162 2.194595 0.204502
F 6.001936 2.012999 -2.126239
F 3.588523 0.831978 -2.140631
C 2.460069 -1.733643 -0.700119
C 3.302561 -2.691875 -0.105983
C 3.734482 -3.862285 -0.739947
C 3.324237 -4.116250 -2.056816
C 2.486521 -3.198439 -2.698603
C 2.082243 -2.038816 -2.016280
F 3.728305 -2.502406 1.166827
F 1.241655 -1.222387 -2.722813
F 2.073725 -3.435448 -3.962282
F 3.722615 -5.234948 -2.690654
F 4.534324 -4.743935 -0.107763
C 1.403610 -0.576160 1.615931
C 1.189939 0.537804 2.447382
C 0.306289 0.562189 3.532380
C -0.402980 -0.600012 3.858518
C -0.207674 -1.749216 3.088831
C 0.701965 -1.722320 2.018013
F 1.820754 1.707768 2.169617
F 0.103251 1.687573 4.254044
F -1.282297 -0.592657 4.884780
F -0.937223 -2.861617 3.347382
F 0.772816 -2.883760 1.307592
C -0.775063 -0.924967 -0.483842
C -2.062916 -1.390895 -0.263576
N -3.133739 -0.530215 -0.185153
C -4.466896 -1.079340 0.052428
C -4.849674 -1.343985 1.387238
C -6.143356 -1.854193 1.594092
C -7.000754 -2.109420 0.516427
C -6.578003 -1.862348 -0.794105
C -5.300951 -1.335945 -1.058777
C -3.909055 -1.076868 2.564155
C -4.061829 -2.110668 3.700626
C -4.858261 -1.106903 -2.503165
C -4.556527 -2.455128 -3.201127
C -2.279858 -2.864655 -0.029668
C -0.901307 2.764428 -1.017946
C -0.783362 2.967449 -2.412307
C -0.515814 4.275200 -2.851408
C -0.365919 5.326297 -1.940632
C -0.443247 5.079634 -0.565045

C -0.697599 3.788708 -0.067899
C -0.941951 1.848119 -3.441870
C 0.307503 1.734421 -4.346921
C -0.699204 3.517470 1.436126
C 0.414532 4.302319 2.166334
C -2.221652 2.057382 -4.286255
C -2.062471 3.834930 2.091210
C -4.102064 0.357584 3.109439
C -5.895695 -0.297937 -3.311874
H -0.427249 4.464269 -3.922318
H -0.167731 6.337219 -2.302103
H -0.286580 5.897002 0.138927
H -1.043378 0.882996 -2.926582
H 0.203835 0.866616 -5.017028
H 0.424961 2.636379 -4.968389
H 1.224412 1.604497 -3.752952
H -2.347473 1.223872 -4.996886
H -3.118042 2.121762 -3.648450
H -2.154823 2.994132 -4.862346
H -0.499952 2.446926 1.582601
H 0.506980 3.927780 3.193835
H 1.384082 4.180802 1.664163
H 0.173021 5.376294 2.210691
H -2.021978 3.587422 3.164009
H -2.300174 4.905551 1.982454
H -2.886266 3.268321 1.631726
H -6.477416 -2.064540 2.610032
H -7.999415 -2.510653 0.699885
H -7.246451 -2.073528 -1.629624
H -3.921595 -0.528197 -2.502431
H -5.495981 -0.086405 -4.316490
H -6.831778 -0.865685 -3.434965
H -6.124220 0.653689 -2.810505
H -4.224952 -2.277610 -4.236871
H -3.767061 -3.017068 -2.678269
H -5.461590 -3.082906 -3.231477
H -2.871528 -1.149697 2.207217
H -3.258012 -1.968839 4.432802
H -5.025266 -1.991136 4.220973
H -4.003255 -3.139332 3.312379
H -3.374052 0.555629 3.910374
H -3.967852 1.115628 2.319002
H -5.120404 0.480668 3.511783
H -1.394854 -3.427346 -0.350108
H -2.420659 -3.043339 1.048785
H -3.175924 -3.233087 -0.546422
H 0.001263 -1.675702 -0.526318
H 1.362847 0.794378 -1.710007
H 1.242551 1.760891 -0.260183
H -4.776918 2.925045 0.450411

81-PH(TS)
C -3.928534 -0.828248 -0.797767
C -3.290241 0.258442 -0.162010
C -3.288879 1.565825 -0.692898
C -4.004759 1.781534 -1.883413

C -4.672587 0.731019 -2.524019
C -4.624697 -0.561601 -1.990038
N -2.627408 0.022161 1.095913
C -1.327595 -0.415551 1.256699
N -1.166450 -0.490127 2.638947
C -2.347145 -0.151290 3.298569
C -3.252697 0.176352 2.334492
C -0.029742 -1.201287 3.181739
N 1.190794 -0.643077 2.643654
C 1.335014 -0.518414 1.265125
N 2.679387 -0.246255 1.093472
C 3.341740 -0.252216 2.322875
C 2.418589 -0.511329 3.291192
C 3.323246 0.059080 -0.160810
C 3.605627 1.413520 -0.456871
C 4.265381 1.683546 -1.666773
C 4.625270 0.646923 -2.538754
C 4.333605 -0.681600 -2.214818
C 3.672637 -1.006842 -1.016764
C 3.131852 2.536214 0.465682
C 1.658613 2.881151 0.142935
C 3.403213 -2.465271 -0.653168
C 2.830233 -3.276089 -1.836278
Si -0.018814 -1.028236 0.042088
P 0.083891 -0.417809 -2.059928
C -2.517983 2.711058 -0.044318
C -3.485075 3.770849 0.531357
C -3.856411 -2.254316 -0.260494
C -5.258363 -2.772289 0.133262
C -1.528584 3.343375 -1.049345
C -3.182492 -3.188490 -1.292765
C 4.696527 -3.116145 -0.107414
C 4.009693 3.802803 0.402906
H 4.405017 -0.051861 2.381061
H 2.513890 -0.603241 4.367590
H 4.613207 -1.481642 -2.901387
H 5.132680 0.879351 -3.477598
H 4.491840 2.715225 -1.937228
H 3.165748 2.169712 1.503734
H 1.281618 3.638256 0.851976
H 1.581913 3.287637 -0.877098
H 1.018693 1.988559 0.189530
H 3.684010 4.514567 1.178225
H 5.074125 3.567854 0.564974
H 3.912114 4.308596 -0.571222
H 2.649611 -2.495783 0.147049
H 2.573797 -4.291294 -1.491903
H 1.923940 -2.796071 -2.236461
H 3.567224 -3.376003 -2.650278
H 4.506502 -4.165110 0.174786
H 5.487392 -3.101840 -0.875707
H 5.070524 -2.577530 0.778902
H -0.099030 -2.266030 2.838551
H -0.027563 -1.128637 4.276033
H -2.423458 -0.163531 4.380109
H -4.277400 0.522223 2.399907

H -5.120561 -1.384094 -2.508289
H -5.216629 0.917141 -3.452632
H -4.018447 2.781649 -2.319321
H -1.924795 2.305790 0.788200
H -2.916160 4.588996 1.003143
H -4.107604 4.203237 -0.269318
H -4.157394 3.330725 1.286291
H -0.935773 4.124166 -0.546740
H -0.846523 2.576988 -1.448682
H -2.066219 3.811002 -1.890363
H -3.230707 -2.260071 0.643489
H -5.185200 -3.797227 0.532764
H -5.721376 -2.129196 0.899841
H -5.926941 -2.794693 -0.742903
H -3.068652 -4.197919 -0.863906
H -3.798550 -3.271494 -2.203537
H -2.190565 -2.803125 -1.578160
H -1.256270 0.103977 -2.006339

82-PH(TS)
C 3.030531 -1.261803 0.060422
C 2.464722 0.020920 0.221000
C 3.197498 1.213873 0.062770
C 4.560918 1.095329 -0.260985
C 5.157855 -0.161112 -0.420313
C 4.396317 -1.326517 -0.264978
N 1.081479 0.103066 0.624811
C -0.000002 0.130161 -0.231678
N -1.081481 0.103096 0.624813
C -0.683236 0.068432 1.953152
C 0.683236 0.068412 1.953150
C -2.464727 0.020969 0.221008
C -3.197458 1.213936 0.062672
C -4.560887 1.095415 -0.261058
C -5.157873 -0.161018 -0.420263
C -4.396379 -1.326439 -0.264824
C -3.030589 -1.261748 0.060563
C -2.551575 2.590871 0.179463
C -3.246727 3.457975 1.252490
C -2.207884 -2.542502 0.175981
C -2.790613 -3.502007 1.237169
P -0.000009 0.025066 -2.056541
C 2.551671 2.590821 0.179708
C 2.550960 3.292752 -1.197888
C 2.207788 -2.542541 0.175731
C 2.097631 -3.230594 -1.204786
C 3.246845 3.457772 1.252845
C 2.790418 -3.502086 1.236937
C -2.097620 -3.230596 -1.204507
C -2.550824 3.292644 -1.198215
H -1.405603 0.042151 2.760771
H 1.405604 0.042116 2.760767
H -4.860450 -2.303924 -0.407971
H -6.217706 -0.232519 -0.674413
H -5.153146 2.001991 -0.398048
H 4.860343 -2.304011 -0.408220

H 6.217684 -0.232629 -0.674479
H 5.153210 2.001896 -0.397897
H -1.501626 2.462797 0.481454
H -2.748660 4.438471 1.327105
H -4.303550 3.632851 0.993673
H -3.214092 2.971558 2.241130
H -2.029400 4.262023 -1.130003
H -2.041932 2.661209 -1.942074
H -3.582395 3.478602 -1.539937
H -1.187379 -2.281229 0.492103
H -2.159996 -4.402614 1.316786
H -2.840817 -3.020407 2.227425
H -3.808044 -3.823853 0.961976
H -1.454648 -4.123471 -1.129955
H -3.092171 -3.550059 -1.557647
H -1.666910 -2.535744 -1.941258
H 1.187261 -2.281256 0.491771
H 2.159789 -4.402692 1.316471
H 3.807870 -3.823927 0.961816
H 2.840543 -3.020522 2.227214
H 1.454599 -4.123432 -1.130325
H 1.667036 -2.535696 -1.941561
H 3.092201 -3.550107 -1.557830
H 1.501712 2.462754 0.481672
H 2.748830 4.438287 1.327554
H 3.214160 2.971251 2.241432
H 4.303684 3.632617 0.994071
H 2.029585 4.262149 -1.129568
H 3.582540 3.478698 -1.539589
H 2.042040 2.661426 -1.941820
H 0.000009 1.458194 -2.195226

83-PH(TS)
C -1.378419 2.056796 -0.517286
C -0.183103 1.660302 0.111752
C 0.886477 2.573127 0.228760
C 0.756991 3.870972 -0.283077
C -0.437762 4.266679 -0.908882
C -1.502723 3.360246 -1.023757
P 0.004301 -0.011413 0.846215
P 0.023158 -0.021652 2.971366
C 1.544841 -0.690556 0.081672
C 2.297725 -1.643589 0.794327
C 3.451567 -2.198024 0.222949
C 3.872730 -1.791793 -1.054511
C 3.134360 -0.830548 -1.761896
C 1.970357 -0.283363 -1.199557
C -1.339852 -1.028880 0.060599
C -1.253574 -1.480867 -1.272667
C -2.317455 -2.193972 -1.842679
C -3.471750 -2.462126 -1.087190
C -3.557505 -2.019240 0.241684
C -2.493633 -1.306076 0.816672
H 1.811253 2.264052 0.719268
H 1.587823 4.573820 -0.192798
H -0.537053 5.279561 -1.305003

H -2.432941 3.664853 -1.507925
H -2.205358 1.351396 -0.608847
H -0.355086 -1.287355 -1.860031
H -2.243472 -2.544896 -2.874431
H -4.297786 -3.020986 -1.532739
H -4.449119 -2.233868 0.834914
H -2.535911 -0.969193 1.856041
H 1.402938 0.470557 -1.747944
H 3.464743 -0.501537 -2.749660
H 4.778952 -2.215848 -1.492288
H 4.029504 -2.937884 0.780797
H 1.993881 -1.927171 1.804481
H -0.299861 1.375946 2.970972

84-PH(TS)
C -1.675962 -2.273421 -0.081586
C -1.477862 -0.744867 -0.221017
C -2.777697 0.017055 0.133530
C -3.953114 -0.467730 -0.741344
C -4.159296 -1.988721 -0.595539
C -2.865269 -2.751880 -0.943661
P -0.024950 -0.131408 0.785565
P -0.293021 -0.260063 2.894051
C 1.437003 -1.161138 0.192368
C 1.704456 -1.139913 -1.329332
C 2.836770 -2.128432 -1.689383
C 4.125768 -1.801080 -0.907345
C 3.862959 -1.780523 0.613028
C 2.722265 -0.804562 0.974890
C 0.389390 1.597767 0.113969
C -0.131294 2.730866 1.026421
C 0.377899 4.100538 0.528988
C -0.021580 4.356786 -0.939193
C 0.457786 3.208160 -1.849254
C -0.066766 1.844468 -1.347335
H -1.223029 -0.526753 -1.272067
H -3.009821 -0.156457 1.196494
H -2.632837 1.101929 0.014039
H -4.871455 0.074658 -0.462185
H -3.742224 -0.229021 -1.800130
H -4.442964 -2.214777 0.448020
H -4.987171 -2.327987 -1.239980
H -3.007758 -3.836622 -0.807018
H -2.625243 -2.586987 -2.010186
H -1.861283 -2.513856 0.978350
H -0.760431 -2.806826 -0.382361
H 1.494324 1.635984 0.127763
H -1.235144 2.718881 1.019203
H 0.171538 2.549372 2.067639
H -0.012568 4.902028 1.177703
H 1.480069 4.124162 0.612468
H -1.122482 4.429753 -1.006029
H 0.389542 5.318386 -1.288962
H 0.127470 3.374475 -2.888460
H 1.562911 3.185011 -1.857987
H -1.168618 1.852071 -1.385524

H 0.273446 1.042107 -2.017405
H 1.152980 -2.186964 0.485662
H 3.037242 0.223174 0.718584
H 2.516719 -0.834907 2.056784
H 4.780530 -1.501434 1.157005
H 3.581939 -2.795175 0.947685
H 4.493013 -0.807353 -1.223453
H 4.915329 -2.531215 -1.150855
H 3.027361 -2.101943 -2.775377
H 2.509634 -3.153975 -1.439928
H 2.013255 -0.123863 -1.627831
H 0.790397 -1.387350 -1.893893
H -1.557832 -0.916699 2.698757

2.5. Palladium complexes

1-Pd
C 1.824953 -3.487490 -0.131086
C 1.924214 -2.263846 0.576665
C 3.173482 -1.808265 1.075709
C 4.313457 -2.601505 0.859426
C 4.229911 -3.819387 0.172644
C 2.992800 -4.250669 -0.317999
N 0.748198 -1.438904 0.795400
Si -0.198448 -1.797686 2.284332
C -0.693235 -0.173161 3.128021
C 3.313324 -0.451297 1.763247
C 4.180653 -0.500704 3.039700
C 0.511080 -3.988019 -0.723297
C 0.584327 -4.038699 -2.266308
Si 0.461020 -0.295275 -0.484118
B -0.942333 1.082543 -0.034684
N -2.394048 1.063623 -0.074280
C -3.284717 -0.046688 -0.236640
C -3.247539 -0.786612 -1.453028
C -4.093995 -1.904732 -1.566666
C -4.980384 -2.257243 -0.539945
C -5.034822 -1.488056 0.625271
C -4.184351 -0.380815 0.807289
C -2.400123 -0.326647 -2.643090
C -2.126601 -1.420125 -3.692199
C -4.276262 0.418921 2.107742
C -5.573247 1.262907 2.131527
C -2.865069 2.385031 0.018806
C -1.801836 3.235349 0.106505
N -0.615355 2.491027 0.060775
C 0.674955 3.121788 0.017633
C 1.308973 3.481533 1.230282
C 2.558838 4.125785 1.161864
C 3.166081 4.387341 -0.070666
C 2.527953 4.011403 -1.260033
C 1.272021 3.377979 -1.245229
C 0.648421 3.226392 2.582178
C -0.022923 4.518398 3.104915
C 0.558082 3.015928 -2.545923
C 1.519058 2.727639 -3.716866

C -3.049836 0.912565 -3.305388
C -4.217608 -0.483043 3.361548
C -0.439382 4.128492 -2.952526
C 1.636304 2.669375 3.630773
C 3.878088 0.589966 0.767182
C 0.125071 -5.372496 -0.154116
C -1.726926 -2.832706 1.840484
C 0.916945 -2.794276 3.453685
H 0.364103 -3.052656 4.374194
H 1.260162 -3.730397 2.985022
H 1.812904 -2.222501 3.742424
H -1.212932 -0.377808 4.079727
H 0.200791 0.427180 3.354300
H -1.361806 0.436010 2.502381
H -2.339929 -3.033615 2.736390
H -2.370871 -2.324441 1.106830
H -1.431295 -3.804675 1.417686
H 5.280145 -2.254696 1.229809
H 5.125831 -4.424520 0.015333
H 2.923999 -5.192338 -0.867252
H 2.309385 -0.113608 2.057732
H 3.912683 1.590788 1.226764
H 4.898598 0.301929 0.462528
H 3.254553 0.642673 -0.141557
H 4.161528 0.481143 3.540773
H 3.816730 -1.263219 3.747155
H 5.231468 -0.732011 2.801300
H -0.281063 -3.277055 -0.455220
H -0.862018 -5.681556 -0.536956
H 0.861053 -6.136959 -0.452727
H 0.084810 -5.357480 0.947079
H -0.378742 -4.379150 -2.684052
H 0.811532 -3.034855 -2.664983
H 1.371208 -4.736172 -2.598736
H -1.783657 4.317067 0.194137
H -3.927570 2.602723 0.011222
H -4.074289 -2.499809 -2.479605
H -5.631474 -3.126694 -0.654953
H -5.732293 -1.756694 1.420601
H -1.409073 -0.010350 -2.287882
H -2.414254 1.269446 -4.133223
H -4.041942 0.654477 -3.713335
H -3.169136 1.732799 -2.582278
H -1.403020 -1.033831 -4.426874
H -1.694236 -2.320537 -3.229329
H -3.043527 -1.705641 -4.235935
H -3.423590 1.109802 2.156802
H -5.625597 1.859592 3.057491
H -5.625468 1.948486 1.271436
H -6.457558 0.605689 2.092923
H -4.196193 0.143070 4.268509
H -5.102733 -1.136313 3.425137
H -3.321681 -1.117159 3.350253
H 3.014968 4.211200 -2.215000
H 4.140729 4.879393 -0.106891
H 3.060182 4.419017 2.085770

H -0.141906 2.477914 2.438743
H -0.509133 4.331682 4.077331
H 0.726599 5.316298 3.238280
H -0.786818 4.877653 2.397695
H 1.091511 2.400412 4.550203
H 2.151826 1.773006 3.253752
H 2.400723 3.415496 3.901624
H -0.011288 2.092423 -2.364932
H -0.960065 3.845784 -3.882972
H -1.196502 4.293794 -2.172809
H 0.096884 5.076435 -3.129353
H 0.953280 2.287519 -4.553132
H 2.002195 3.649098 -4.084997
H 2.308678 2.019407 -3.411325
Pd 1.526867 -0.376000 -2.356705

2-Pd
C 2.019274 1.866463 -2.337072
Si 2.850413 0.865366 -0.941035
C 4.340311 1.855973 -0.271583
C 3.456100 -0.777675 -1.680660
C 1.563463 0.597001 0.459651
Si -0.000057 -0.265344 -0.172219
C -1.493767 0.533529 0.679043
Si -2.000442 2.135466 -0.266456
C -3.727045 2.756230 0.256252
Si 2.232004 -0.270504 2.043060
C 3.361264 -1.740998 1.620957
C 3.165738 1.027263 3.082524
C 0.788550 -0.936648 3.101310
Si -2.929806 -0.732024 0.896795
C -4.138247 -0.095327 2.230861
C -3.806590 -0.981108 -0.772906
C -2.291676 -2.430877 1.482242
C -0.743783 3.511996 0.152065
C -2.004038 1.842940 -2.148485
H 1.250869 1.595161 0.827721
H -1.167453 0.889826 1.677278
H 3.964482 -0.593811 -2.643716
H 4.159296 -1.308892 -1.021003
H 2.594629 -1.443787 -1.870308
H 5.011938 2.151141 -1.097076
H 4.020120 2.777734 0.244122
H 4.936210 1.263581 0.443406
H 2.740896 2.097085 -3.140613
H 1.197717 1.281150 -2.785500
H 1.598514 2.823243 -1.983277
H 3.528194 0.584294 4.026884
H 4.034091 1.441427 2.546081
H 2.502176 1.870093 3.344139
H 3.572020 -2.335085 2.527378
H 2.877891 -2.403435 0.883628
H 4.326737 -1.417082 1.199325
H 1.169058 -1.332712 4.059504
H 0.043501 -0.157268 3.334810
H 0.260281 -1.759008 2.591619

H -3.944693 3.715208 -0.246875
H -4.523381 2.045713 -0.018246
H -3.789577 2.925976 1.344090
H -2.295396 2.765182 -2.682104
H -1.010564 1.540665 -2.518540
H -2.710249 1.046780 -2.431690
H -1.055132 4.470966 -0.298405
H -0.662173 3.669354 1.242010
H 0.263829 3.279366 -0.228472
H -3.126176 -3.153257 1.530302
H -1.537293 -2.824747 0.777933
H -1.837324 -2.379848 2.485839
H -4.901869 -0.862039 2.452145
H -3.605164 0.116258 3.174846
H -4.661294 0.824436 1.929031
H -4.575029 -1.770646 -0.703724
H -4.295024 -0.064213 -1.142165
H -3.057634 -1.296467 -1.522340
Pd -0.138346 -1.880573 -1.592941

3-Pd
C 3.452790 -1.743859 -1.620797
Si 2.830204 -0.086908 -0.907769
C 4.263645 0.691482 0.073554
N 1.384132 -0.373992 0.117953
Si -0.039188 0.639741 -0.102850
N -1.444469 -0.399548 -0.173009
Si -2.950121 0.142331 0.644320
C -4.196488 0.880888 -0.586018
C 2.405093 1.064336 -2.359732
Si 1.597342 -1.103767 1.743076
C -0.071371 -1.536068 2.546129
C 2.669481 -2.673305 1.638490
C 2.419727 0.145425 2.924539
Si -1.434958 -1.826849 -1.256009
C -0.861390 -3.419915 -0.389768
C -3.174107 -2.126827 -1.979700
C -0.318935 -1.495954 -2.760750
C -3.698285 -1.353786 1.561016
C -2.594207 1.479872 1.950951
H 1.594700 0.669921 -2.993378
H 2.090032 2.059607 -2.003518
H 3.301325 1.182790 -2.995791
H 2.661735 -2.302267 -2.147084
H 4.258229 -1.544746 -2.350728
H 3.865036 -2.406910 -0.844392
H 3.945167 1.615124 0.584174
H 4.672228 0.006375 0.834762
H 5.088365 0.950200 -0.614184
H 0.126564 -2.089965 3.481538
H -0.637788 -0.630832 2.815222
H -0.716547 -2.148516 1.905743
H 2.681396 -3.172465 2.623633
H 2.285640 -3.395176 0.899209
H 3.714419 -2.443407 1.373194
H 2.377590 -0.225277 3.964560

H 3.473290 0.349849 2.681264
H 1.877933 1.106668 2.886457
H -0.882488 -4.262422 -1.104112
H 0.167657 -3.323619 -0.010312
H -1.512831 -3.686987 0.458900
H -3.142703 -3.047816 -2.588871
H -3.967528 -2.254016 -1.228293
H -3.470062 -1.299601 -2.645240
H -0.434604 -2.312327 -3.495779
H -0.601691 -0.554121 -3.261550
H 0.743929 -1.433545 -2.495141
H -5.046272 1.330921 -0.042420
H -3.714445 1.680423 -1.174649
H -4.601475 0.137135 -1.288742
H -4.665283 -1.074677 2.016088
H -3.876825 -2.227399 0.914310
H -3.025780 -1.673772 2.373811
H -3.519101 1.661594 2.529541
H -1.803914 1.199156 2.666254
H -2.282875 2.425965 1.477857
Pd -0.052659 2.790685 -0.228156

4-Pd
C 1.344151 3.115657 -0.551086
C 0.255376 3.258189 0.350876
C 0.509948 3.441234 1.736711
C 1.832677 3.390804 2.200225
C 2.917238 3.164112 1.335325
C 2.652891 3.046853 -0.037223
C -1.156050 3.244020 -0.147960
C -2.050759 2.171118 0.132423
C -3.381922 2.205259 -0.347423
C -3.806767 3.311699 -1.110173
C -2.933928 4.367282 -1.400529
C -1.619473 4.327431 -0.918779
S -1.518240 0.762959 1.136853
Si 0.000068 0.000148 -0.221246
S 1.518153 -0.762802 1.136980
C 2.050531 -2.170833 0.132281
C 3.381640 -2.204947 -0.347705
C 3.806331 -3.311247 -1.110754
C 2.933399 -4.366723 -1.401233
C 1.619009 -4.326927 -0.919290
C 1.155718 -3.243643 -0.148208
C 4.379472 -1.121514 -0.074670
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7-Pd

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H -4.685541 0.850901 0.705001
H -1.866159 -2.809319 -2.215533
H -0.624894 -2.233096 -1.075567
H -1.939873 -3.344655 -0.502559
H -3.906116 -1.658430 -2.444556
H -4.469995 -2.196536 -0.831517
H -4.418950 -0.448336 -1.237718
H -2.564277 2.417794 -2.173632
H -0.933465 1.661133 -1.925164
H -2.314069 0.662751 -2.448216
H -3.013163 3.252055 0.001987

H -2.596894 2.273539 1.447869
H -1.289585 2.890740 0.401030
Pd 1.171839 -0.269890 -1.964007

8-Pd
C 1.197045 -2.512705 0.775879
O 0.239142 -1.474535 1.151238
C 0.659609 -0.999665 2.468944
C 2.204056 -1.109520 2.492580
C 2.549325 -1.952420 1.228353
Si -0.204463 -0.097464 -0.441760
O -0.596080 1.141181 0.639679
C 0.029112 2.452571 0.718745
C 1.510365 2.315182 1.120406
O -1.641054 -0.853560 -0.802978
C -2.972519 -0.778677 -0.221719
C -2.924779 -0.986786 1.304988
C -3.769712 -1.913469 -0.887494
C -3.589357 0.590332 -0.564256
C -0.095466 3.170173 -0.639203
C -0.753262 3.212386 1.802794
H -4.626044 0.645234 -0.191994
H -2.997487 1.391517 -0.100365
H -3.597348 0.734792 -1.656075
H -4.808129 -1.915743 -0.517853
H -3.779313 -1.778192 -1.979912
H -3.307766 -2.886399 -0.657336
H -3.950934 -1.004372 1.707711
H -2.433867 -1.942414 1.542768
H -2.369677 -0.169001 1.785542
H 1.981106 3.309933 1.179701
H 1.595802 1.828079 2.104451
H 2.041721 1.705428 0.370285
H -0.336047 4.223982 1.932567
H -1.813512 3.299258 1.517903
H -0.690418 2.678449 2.764913
H 0.314044 4.191239 -0.569895
H 0.459456 2.609190 -1.409679
H -1.153911 3.231394 -0.938366
H 0.266322 0.017834 2.562056
H 0.187045 -1.657793 3.215614
H 2.540361 -1.601049 3.417840
H 2.671765 -0.116750 2.438866
H 3.282558 -2.747371 1.430731
H 2.926413 -1.295541 0.426413
H 0.911550 -3.437057 1.305420
H 1.112152 -2.633090 -0.312780
Pd 1.525088 -0.103177 -1.754076

9-Pd
C -3.114423 0.970728 1.227997
C -2.087741 1.681495 0.557798
C -2.399029 2.396433 -0.630634
C -3.681631 2.268901 -1.191560
C -4.676576 1.473183 -0.597123
C -4.380717 0.855560 0.627643

C -0.709074 1.793339 1.144738
C 0.431804 1.119466 0.600598
C 1.704083 1.427809 1.173367
C 1.809975 2.313418 2.266242
C 0.675317 2.916988 2.818070
C -0.575935 2.664282 2.244685
Si 0.359888 -0.304498 -0.734374
Cl -0.011459 0.687950 -2.630747
C 2.997168 0.895273 0.626120
C 3.567947 1.515157 -0.513873
C 4.778974 1.022213 -1.027138
C 5.448668 -0.061042 -0.434841
C 4.895130 -0.626806 0.726394
C 3.685781 -0.161315 1.273218
C 2.893279 2.698197 -1.181892
C 6.732019 -0.604636 -1.032659
C 3.118453 -0.845836 2.501794
C -1.424358 3.390727 -1.233259
C -6.025580 1.285384 -1.263374
C -2.910220 0.375404 2.608301
C -1.327910 -1.150247 -0.272791
N -2.464563 -1.452187 -0.971066
C -3.295355 -2.290685 -0.226625
C -2.653618 -2.532749 0.961342
N -1.455615 -1.822202 0.917725
C -2.781076 -0.969229 -2.319111
C -0.389350 -1.921661 1.910970
C -3.070883 -3.360770 2.135322
C -4.642421 -2.741773 -0.697312
H 0.468133 -2.448805 1.446627
H -0.049431 -0.918970 2.197169
H -0.766074 -2.452678 2.793207
H -4.072709 -3.777599 1.961585
H -2.379880 -4.203079 2.310472
H -3.106795 -2.760339 3.060589
H -4.581122 -3.333452 -1.626510
H -5.112861 -3.369912 0.071936
H -5.306270 -1.881227 -0.887652
H -2.769823 0.124521 -2.326827
H -2.041161 -1.352992 -3.033907
H -3.780518 -1.328331 -2.589526
H 2.801351 2.525119 2.673848
H 0.766636 3.594062 3.670803
H -1.469731 3.156701 2.635823
H 5.210084 1.501729 -1.910991
H 5.418247 -1.448445 1.225330
H 3.576447 3.178430 -1.899824
H 1.990961 2.384578 -1.730147
H 2.577174 3.449179 -0.439407
H 7.349902 -1.103705 -0.268594
H 6.517396 -1.347049 -1.822197
H 7.330560 0.198157 -1.493569
H 2.596143 -0.140179 3.165256
H 2.390125 -1.613905 2.188219
H 3.915541 -1.346738 3.074307
H -3.908260 2.811359 -2.114486

H -5.156539 0.275813 1.137053
H -1.865899 0.095347 2.788325
H -3.182963 1.108944 3.388203
H -3.549447 -0.509654 2.748977
H -6.781623 0.931606 -0.543983
H -6.387626 2.225448 -1.711237
H -5.968166 0.542056 -2.079957
H -1.630477 3.544109 -2.302982
H -1.529073 4.365225 -0.721537
H -0.381930 3.071356 -1.123837
Pd 1.954589 -1.805247 -0.722340

10-Pd
N -1.287906 -2.606118 0.035820
C -1.253249 -1.498065 -0.781102
N -2.404090 -1.589868 -1.522240
C -3.151853 -2.710498 -1.157186
C -2.446655 -3.349934 -0.173371
Si 0.359457 -0.379511 -0.925331
Cl -0.047654 0.912176 -2.638666
C -2.813328 -0.681915 -2.598661
C -4.488279 -3.038780 -1.742805
C -2.761179 -4.583243 0.612274
C -0.191289 -3.128470 0.852701
C 0.235918 0.856491 0.609673
C -0.962154 1.312633 1.237205
C -0.923830 2.177083 2.351305
C 0.289916 2.599518 2.898112
C 1.478963 2.164437 2.306740
C 1.471940 1.326349 1.174552
C -2.346645 0.948727 0.779947
C -3.077314 -0.109455 1.379140
C -4.374490 -0.381673 0.894723
C -5.007921 0.412443 -0.067586
C -4.301865 1.515871 -0.572959
C -2.979859 1.786887 -0.187273
C -2.656586 -0.983570 2.580519
C -1.196698 -0.972190 3.080732
C -2.270436 3.027156 -0.741927
C -2.624205 3.354562 -2.208369
C -6.456106 0.137526 -0.462375
C -7.399100 1.087409 0.315921
C 2.811398 0.957905 0.606049
C 3.540624 1.830992 -0.221783
C 4.731443 1.349199 -0.835963
C 5.200165 0.048297 -0.662592
C 4.500267 -0.809745 0.226896
C 3.312656 -0.379032 0.887839
C 3.194077 3.299850 -0.521147
C 1.712404 3.672732 -0.751920
C 6.429212 -0.458433 -1.401567
C 6.064859 -1.654637 -2.312775
C 2.841163 -1.108302 2.158561
C 3.088228 -2.630433 2.145158
C 3.817183 4.225806 0.554395
C 7.562865 -0.845823 -0.423413

C 3.537501 -0.486421 3.392516
C -2.589327 4.255683 0.145199
C -6.716249 0.259555 -1.979528
C -3.567401 -0.639913 3.791658
H 0.632571 -2.409282 0.866560
H -0.550148 -3.321823 1.871608
H 0.178556 -4.060859 0.397081
H -3.723422 -5.001621 0.286189
H -1.988529 -5.360094 0.483003
H -2.830321 -4.364029 1.692473
H -5.221864 -2.245737 -1.522421
H -4.441281 -3.162636 -2.837682
H -4.861597 -3.978252 -1.311716
H -2.671878 0.349066 -2.276977
H -2.216284 -0.875236 -3.500658
H -3.875939 -0.845661 -2.804335
H 2.439393 2.486039 2.710459
H 0.309299 3.256220 3.770961
H -1.868451 2.494785 2.798076
H 5.282341 2.020852 -1.500810
H 4.936798 -1.772794 0.491588
H 3.711445 3.532864 -1.468088
H 6.797761 0.360935 -2.043000
H 1.759753 -0.936777 2.262343
H -4.786551 2.169837 -1.298616
H -4.923638 -1.227669 1.319946
H -2.890786 -2.021968 2.283367
H -6.695072 -0.897200 -0.156670
H -1.187785 2.849601 -0.699727
H 1.673361 4.688385 -1.182294
H 1.230779 2.979382 -1.452927
H 1.133962 3.682557 0.181307
H 3.717038 5.282093 0.250024
H 3.300967 4.099802 1.518305
H 4.886419 4.001737 0.699673
H 2.594485 -3.096877 3.014081
H 2.702795 -3.090487 1.220659
H 4.164714 -2.858785 2.214735
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H 4.630197 -0.607317 3.307026
H 3.313577 0.586249 3.474578
H 6.948506 -2.001804 -2.875223
H 5.688369 -2.495041 -1.706341
H 5.274619 -1.371684 -3.026193
H 8.454550 -1.183066 -0.978326
H 7.845158 0.009571 0.211134
H 7.241082 -1.668745 0.236316
H -2.070845 5.147970 -0.244310
H -3.674685 4.454921 0.142456
H -2.267479 4.094028 1.183688
H -1.973575 4.170110 -2.561586
H -2.468379 2.488443 -2.866932
H -3.668142 3.696978 -2.308238
H -8.454510 0.878727 0.071925
H -7.256912 0.974504 1.402257
H -7.181045 2.135050 0.050734

H -7.765871 0.011517 -2.206559
H -6.531333 1.287353 -2.329935
H -6.067618 -0.416587 -2.558931
H -3.342218 -1.309212 4.639455
H -3.381155 0.397939 4.113369
H -4.635147 -0.734920 3.543067
H -1.057130 -1.828698 3.762245
H -0.466088 -1.043297 2.271800
H -0.969885 -0.054482 3.639206
Pd 2.390184 -1.328707 -0.909325

11-Pd
C 2.781079 1.603244 0.892059
C 2.105727 1.251265 -0.288508
C 2.763552 0.734054 -1.427876
C 4.147217 0.518601 -1.331816
C 4.861589 0.815350 -0.153210
C 4.168327 1.370416 0.934245
N 0.680291 1.490003 -0.383726
C -0.330146 0.614562 -0.077368
N -1.475473 1.288172 -0.408024
C -1.182875 2.551634 -0.908105
C 0.175629 2.679076 -0.889377
C -2.846782 0.830868 -0.318366
C -3.567276 1.075069 0.864481
C -4.910937 0.663650 0.893730
C -5.520958 0.041036 -0.208437
C -4.764552 -0.152749 -1.378785
C -3.419022 0.234939 -1.459285
C -2.928403 1.748986 2.059267
C -2.601084 -0.021459 -2.706543
C -6.959680 -0.429970 -0.133420
Si 0.072328 -1.236426 0.586441
Cl -1.769261 -2.241015 0.102331
C 1.996653 0.396733 -2.688917
C 6.348649 0.533747 -0.065853
C 2.048152 2.168541 2.088684
Cl -0.225793 -0.798667 2.709471
H 1.401730 1.253292 -3.048979
H 2.760222 2.609670 2.801989
H -1.847491 -0.802031 -2.510551
H -2.199463 1.078365 2.541234
H 2.686115 0.089221 -3.488872
H 1.485237 1.375031 2.606430
H -3.246619 -0.364663 -3.528327
H -3.693768 2.022178 2.800864
H 0.836076 3.486085 -1.183526
H -1.972741 3.223332 -1.223262
H 4.676349 0.110930 -2.197176
H 4.714460 1.625188 1.845931
H -5.228118 -0.627083 -2.247613
H -5.492033 0.836688 1.803163
H 1.322152 2.943949 1.793748
H 1.304183 -0.439006 -2.484378
H -2.063524 0.882123 -3.038943
H -2.386283 2.663181 1.765056

H -7.535116 0.155555 0.600838
H -7.458709 -0.350956 -1.112581
H -7.006589 -1.488975 0.176046
H 6.814454 1.095552 0.758464
H 6.533436 -0.539725 0.115229
H 6.862355 0.799970 -1.004183
Pd 2.022046 -1.901437 -0.112799

12-Pd
C 3.178855 1.466594 0.080609
C 2.800181 0.161246 0.474884
C 3.670398 -0.946197 0.455213
C 4.989310 -0.713685 0.020276
C 5.403297 0.562894 -0.372997
C 4.506426 1.640044 -0.343291
N 1.465290 -0.016629 1.015134
C 0.289648 -0.107579 0.323635
N -0.680407 -0.086952 1.288976
C -0.120481 -0.005076 2.555338
C 1.232486 0.042907 2.382504
Si -0.182370 -0.466481 -1.589709
Cl 0.523509 -2.537035 -1.505310
C -2.111047 0.085190 1.102979
C -2.944758 -1.052255 1.062599
C -4.330696 -0.824616 0.982133
C -4.850215 0.476652 0.935053
C -3.989275 1.582370 0.973860
C -2.596554 1.413009 1.070105
C -2.387172 -2.470136 1.055118
C -2.722417 -3.197017 2.377780
C -1.670330 2.625782 1.048214
C -2.007789 3.628695 2.173539
C 3.240634 -2.330902 0.934081
C 3.714104 -3.456576 -0.010663
C 2.201865 2.642156 0.135312
C 2.451743 3.700186 -0.958269
Cl 1.445643 0.506837 -2.607345
C -2.900512 -3.260439 -0.168539
C -1.712621 3.305691 -0.340255
C 3.760596 -2.579646 2.370937
C 2.225040 3.306365 1.533916
H -0.743365 0.033011 3.440706
H 2.052089 0.124659 3.085266
H -5.003837 -1.681766 0.937220
H -5.929320 0.629300 0.865084
H -4.396209 2.593573 0.923450
H 5.692625 -1.546557 -0.011138
H 6.429459 0.721550 -0.711365
H 4.839114 2.626436 -0.666262
H -0.637221 2.290386 1.214734
H -1.299726 4.473017 2.148053
H -3.024490 4.035095 2.049726
H -1.948196 3.151285 3.165304
H -0.971503 4.121371 -0.386171
H -1.496632 2.570551 -1.135049
H -2.710951 3.733678 -0.529556

H -1.293413 -2.416236 0.962116
H -2.300701 -4.215257 2.367776
H -2.312147 -2.657310 3.247802
H -3.814025 -3.277879 2.510755
H -2.407369 -4.244412 -0.209582
H -3.989863 -3.420870 -0.108833
H -2.668378 -2.707534 -1.093852
H 2.142250 -2.366325 0.950502
H 3.442681 -3.574458 2.724275
H 4.862247 -2.540249 2.391856
H 3.381203 -1.823997 3.078119
H 3.296066 -4.417332 0.329642
H 3.372765 -3.272299 -1.038647
H 4.812616 -3.548611 -0.007415
H 1.189754 2.251113 -0.037093
H 1.490860 4.128345 1.573607
H 1.977980 2.587845 2.330290
H 3.224183 3.723884 1.741552
H 1.631921 4.435717 -0.940806
H 3.393468 4.246763 -0.785028
H 2.484927 3.234564 -1.953256
Pd -2.284994 -0.008822 -1.902303

13-Pd
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C 2.456240 0.529235 0.448188
C 3.034138 1.727235 -0.021673
C 4.384493 1.680843 -0.413736
C 5.112370 0.487039 -0.342434
C 4.501039 -0.689146 0.113892
N 1.083374 0.565039 0.887133
C -0.000029 0.387002 0.065324
N -1.083482 0.564920 0.887080
C -0.682565 0.852756 2.188573
C 0.682375 0.852805 2.188605
C -2.456351 0.529035 0.448158
C -3.152675 -0.697892 0.514127
C -4.501066 -0.689466 0.113777
C -5.112492 0.486720 -0.342411
C -4.384706 1.680590 -0.413610
C -3.034346 1.727037 -0.021585
C -2.481660 -1.964546 1.038778
C -2.748880 -2.123910 2.554134
C -2.249815 3.033292 -0.122910
C -2.851022 4.112892 0.805809
Si 0.000007 -0.302588 -1.741430
C 2.249534 3.033441 -0.123032
C 2.187649 3.528605 -1.585802
C 2.481748 -1.964300 1.039019
C 2.903768 -3.230743 0.268027
H -1.179439 0.454650 -2.293081
C 2.850679 4.113074 0.805691
C 2.748979 -2.123537 2.554392
C -2.187934 3.528429 -1.585688
C -2.903539 -3.230978 0.267679
H 1.407353 1.033971 2.972557

H -1.407598 1.033878 2.972484
H 4.860969 2.590704 -0.783594
H 6.159441 0.469192 -0.652871
H 5.073707 -1.616307 0.151608
H -4.861263 2.590447 -0.783374
H -6.159569 0.468827 -0.652824
H -5.073668 -1.616671 0.151408
H 1.395987 -1.862730 0.879614
H 2.238198 -3.022864 2.937114
H 3.829591 -2.229598 2.749126
H 2.382412 -1.251357 3.119662
H 2.318435 -4.089327 0.635316
H 2.695661 -3.101410 -0.807237
H 3.971682 -3.468116 0.409327
H 1.215518 2.851425 0.204171
H 2.263932 5.043876 0.735639
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H 3.890050 4.340669 0.518143
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H 3.196685 3.760856 -1.963979
H 1.740710 2.759785 -2.233895
H -1.215799 2.851339 0.204334
H -2.264314 5.043719 0.735762
H -3.890406 4.340451 0.518280
H -2.853126 3.777452 1.855802
H -1.578973 4.445736 -1.646728
H -1.740961 2.759614 -2.233766
H -3.196982 3.760609 -1.963876
H -1.395905 -1.862898 0.879375
H -2.238010 -3.023209 2.936804
H -2.382392 -1.251730 3.119457
H -3.829481 -2.230083 2.748866
H -2.318135 -4.089526 0.634934
H -3.971436 -3.468465 0.408901
H -2.695381 -3.101533 -0.807559
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Pd 0.000239 -2.493711 -1.464009

14-Pd
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C -1.976252 3.303297 -0.109017
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C -0.274128 4.996393 -0.258769
C -0.811701 5.621235 0.876215
C -1.917670 5.066779 1.529941
N -2.625658 2.134552 -0.649103
C -2.233653 0.840906 -0.391029
N -3.132877 0.077569 -1.108493
C -4.079471 0.881280 -1.741536
C -3.757609 2.175781 -1.456942
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15-Pd
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C -0.669347 -4.297508 2.349510
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17-Pd
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C 0.439452 4.730230 1.970098
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H 2.003027 1.322376 -2.340276
H 1.004555 0.706687 -4.555995
H 1.839088 -0.874698 -4.478014
H 0.570976 -0.467530 -3.278277
H 3.061742 2.073498 -4.412188

H 4.415982 1.604042 -3.347134
H 3.884389 0.518837 -4.648221
H -0.643935 2.896762 1.487326
H 0.624119 2.707246 2.715697
H -0.283802 5.023819 2.749479
H 1.442380 5.006354 2.343673
H -0.868162 5.278150 0.328957
H 0.234604 6.582127 0.826792
H 0.915161 5.542301 -1.390859
H 2.170561 5.351440 -0.154765
H 0.071593 3.247900 -0.980944
H 1.776539 3.203420 -1.422344
H 0.406585 0.530628 2.677168
H -1.011746 1.439762 3.240582
H 0.320970 0.578146 5.171204
H -1.307239 -0.125757 5.157187
H 1.246068 -1.495863 4.116675
H 0.384435 -1.910280 5.617690
H -0.209658 -3.474167 3.702829
H -1.625138 -2.589077 4.296139
H 0.091942 -1.838651 1.837103
H -1.497468 -2.586104 1.756562
H -5.627473 0.224843 0.709061
H -5.698243 0.001247 2.481319
H -4.728135 1.330671 1.788857
H -4.972078 -2.190333 0.581306
H -3.536258 -2.826047 1.431024
H -4.980587 -2.330805 2.359834
H 5.172533 2.857369 -0.466143
H 4.875452 1.299702 -1.289213
H 3.755122 2.667644 -1.529534
H 5.327878 1.778695 1.716130
H 4.047071 0.678528 2.302866
H 5.102236 0.181475 0.942489
Pd 0.930168 -1.617109 -0.888377

18-Pd

C	-2.659286	-1.798016	-2.377217
C	-1.780302	-0.610975	-2.383942
C	-2.608817	0.501684	-1.834524
C	-3.815334	-0.052242	-1.405448
C	-3.842615	-1.462259	-1.738231
Si	-1.004262	-0.741698	-0.542809
Pd	-1.784067	-1.903014	1.114685
N	0.369846	0.253711	-0.598742
C	1.210569	0.580717	0.336886
N	1.224923	1.762074	1.070104
C	2.343076	1.802676	1.907040
C	3.030681	0.642015	1.722427
N	2.326821	-0.118472	0.783605
C	0.235115	2.791777	0.922269
C	0.522744	3.880119	0.067054
C	-0.465101	4.872123	-0.073449
C	-1.684930	4.772076	0.607211
C	-1.945674	3.674435	1.437594
C	-0.992218	2.654201	1.611836

C	1.823945	3.935965	-0.733204
C	1.631542	3.219255	-2.093023
C	-1.256402	1.460072	2.525217
C	-0.660782	1.712274	3.930137
C	2.757369	-1.369709	0.226414
C	2.425854	-2.571504	0.897717
C	2.894773	-3.773043	0.336051
C	3.640724	-3.776135	-0.850947
C	3.928327	-2.573257	-1.505259
C	3.491199	-1.343388	-0.980015
C	1.602150	-2.561474	2.183296
C	2.518303	-2.412828	3.421410
C	3.803633	-0.046608	-1.722646
C	3.158996	-0.054628	-3.126445
C	0.699724	-3.802491	2.337210
C	5.328336	0.191838	-1.809472
C	-2.744635	1.075534	2.619040
C	2.354030	5.369365	-0.945543
C	-2.210269	-3.150139	-2.858008
C	-4.976717	-2.375969	-1.353032
C	-4.924680	0.649957	-0.670289
C	-2.218049	1.955951	-1.890857
C	-0.771645	-0.361910	-3.500361
H	2.532834	2.656249	2.546255
H	3.953067	0.278584	2.157819
H	-2.906042	3.602479	1.948570
H	-2.440985	5.550756	0.483053
H	-0.281047	5.726708	-0.725653
H	2.595500	3.382257	-0.176277
H	3.348279	5.327611	-1.418599
H	1.694969	5.947198	-1.613573
H	2.441059	5.913441	0.008755
H	2.581014	3.209802	-2.654463
H	1.291373	2.183648	-1.949094
H	0.876304	3.751165	-2.695406
H	-0.750889	0.579675	2.097770
H	-2.828400	0.124257	3.169468
H	-3.336969	1.836836	3.155555
H	-3.167500	0.918149	1.616792
H	-0.826616	0.830712	4.571891
H	0.422864	1.900188	3.875195
H	-1.141848	2.583867	4.405672
H	4.495070	-2.580255	-2.438289
H	3.987643	-4.722650	-1.271783
H	2.658602	-4.719156	0.823531
H	0.927261	-1.691151	2.137747
H	1.910371	-2.384467	4.341213
H	3.211113	-3.268590	3.490370
H	3.113857	-1.488896	3.375240
H	0.042413	-3.662850	3.211174
H	0.069342	-3.932908	1.441637
H	1.286196	-4.722051	2.504467
H	3.368324	0.795999	-1.168083
H	3.350120	0.904193	-3.635852
H	3.579430	-0.863616	-3.746513
H	2.072839	-0.200323	-3.045654

H	5.534410	1.143685	-2.326655
H	5.781560	0.233766	-0.805601
H	5.820775	-0.617359	-2.373282
H	-5.136493	0.149382	0.290940
H	-4.671168	1.699785	-0.459481
H	-5.864759	0.635529	-1.251730
H	-2.849401	2.571178	-1.233271
H	-1.173361	2.101069	-1.578646
H	-2.316285	2.348551	-2.920881
H	-4.783306	-3.415468	-1.656849
H	-5.129698	-2.367935	-0.259505
H	-5.929454	-2.057499	-1.814718
H	-2.994857	-3.908731	-2.717783
H	-1.944940	-3.130494	-3.931145
H	-1.315870	-3.490257	-2.306372
H	-1.291126	-0.132620	-4.448086
H	-0.117125	0.484744	-3.248300
H	-0.134646	-1.245698	-3.663918

19-Pd

C	0.755840	-2.932511	-2.180174
C	1.160224	-1.602444	-2.191374
C	-0.056361	-0.752561	-2.055186
C	-1.201734	-1.704292	-2.105385
C	-0.684897	-2.994713	-2.129325
Si	0.018796	-0.705519	-0.074987
Pd	0.133118	-2.402190	1.255941
C	-0.017432	1.116065	0.571227
C	-1.245751	1.690164	1.008113
C	-1.244671	2.857331	1.796497
C	-0.045099	3.483550	2.155149
C	1.166467	2.949617	1.700455
C	1.194693	1.782873	0.911682
C	-2.582435	1.096919	0.652520
C	-3.336433	1.651826	-0.420566
C	-4.615342	1.139435	-0.689399
C	-5.168862	0.091744	0.063116
C	-4.418847	-0.430552	1.126131
C	-3.140429	0.060461	1.450343
C	-2.813472	2.833095	-1.244729
C	-3.188630	2.758012	-2.743532
C	-2.426095	-0.442495	2.705206
C	-2.684665	-1.931569	3.013562
C	-6.537054	-0.481907	-0.286011
C	-7.640438	0.598979	-0.233180
C	2.541462	1.294803	0.450380
C	3.167146	1.908585	-0.669395
C	4.459793	1.494867	-1.038308
C	5.142754	0.486996	-0.345470
C	4.514594	-0.097725	0.766476
C	3.234867	0.296090	1.191233
C	2.493882	3.044800	-1.445759
C	2.746822	2.989322	-2.970339
C	6.521309	0.019941	-0.795865
C	6.484913	-1.464291	-1.229524
C	2.656913	-0.265822	2.490088

C	3.044472	-1.733998	2.759153
C	2.965374	4.417376	-0.906654
C	7.581798	0.237124	0.307975
C	3.082565	0.628396	3.679307
C	-2.826157	0.431075	3.918667
C	-6.506028	-1.162884	-1.674604
C	-3.338952	4.168310	-0.662879
C	-2.654225	-1.308753	-2.120709
C	-1.462637	-4.279386	-2.041419
C	1.645345	-4.145139	-2.145057
C	2.567447	-1.082982	-2.321478
C	-0.140351	0.607866	-2.735419
H	-2.199680	3.263171	2.135059
H	-0.054436	4.378739	2.780688
H	2.111501	3.428837	1.962519
H	4.946335	1.956669	-1.900201
H	5.043615	-0.874267	1.320576
H	-4.850714	-1.236088	1.722981
H	-5.194076	1.556244	-1.514779
H	-1.342354	-0.335090	2.549071
H	-2.019136	-2.255496	3.830292
H	-3.723584	-2.111058	3.339172
H	-2.478790	-2.552031	2.124393
H	-2.305005	0.082674	4.826558
H	-2.563008	1.486094	3.750110
H	-3.913238	0.366809	4.095388
H	-6.779615	-1.253391	0.465379
H	-7.488693	-1.604086	-1.911752
H	-6.260376	-0.427235	-2.458106
H	-5.743765	-1.957153	-1.704514
H	-8.624751	0.155612	-0.458117
H	-7.685164	1.069619	0.761920
H	-7.445952	1.389855	-0.976318
H	-1.715491	2.845406	-1.168228
H	-2.970057	5.018485	-1.261549
H	-4.441504	4.179796	-0.685367
H	-3.011219	4.307869	0.376610
H	-2.642969	3.537092	-3.299859
H	-2.943620	1.779379	-3.181868
H	-4.265638	2.937869	-2.892674
H	1.559404	-0.238405	2.419108
H	2.456136	-2.116042	3.609346
H	2.829883	-2.357095	1.874006
H	4.112101	-1.838464	3.018031
H	2.653002	0.242138	4.619303
H	4.181455	0.638409	3.777077
H	2.736247	1.663396	3.538319
H	1.407826	2.976090	-1.279904
H	2.110746	3.733247	-3.476693
H	3.794983	3.231794	-3.209320
H	2.523539	1.997047	-3.389106
H	2.484624	5.235859	-1.468945
H	2.717402	4.534464	0.157518
H	4.058070	4.511961	-1.022207
H	6.811990	0.624855	-1.672508
H	7.478320	-1.788460	-1.582328

H	6.195566	-2.105045	-0.380495
H	5.753558	-1.620574	-2.038097
H	8.576708	-0.081119	-0.045684
H	7.634293	1.297474	0.602223
H	7.333001	-0.354153	1.204457
H	3.202827	-1.827857	-2.826938
H	2.597830	-0.156380	-2.915552
H	3.036330	-0.857750	-1.351927
H	1.322303	-4.906410	-2.876452
H	2.694497	-3.886120	-2.352898
H	1.608946	-4.618155	-1.146805
H	-1.126759	-5.008705	-2.799208
H	-1.319019	-4.751088	-1.052256
H	-2.541784	-4.110920	-2.176311
H	-0.178496	0.494070	-3.833116
H	-1.036614	1.149312	-2.409888
H	0.729478	1.224928	-2.479602
H	-3.259077	-2.096706	-2.596971
H	-3.065518	-1.143952	-1.113188
H	-2.809095	-0.377519	-2.687061

20-Pd

C	-2.101696	1.124817	-1.025577
C	-1.527929	1.488189	0.301571
C	-2.177017	0.566192	1.267938
C	-2.938350	-0.345269	0.555863
C	-2.893150	0.000926	-0.857408
Si	0.120595	0.298104	0.041947
Pd	-0.087189	-1.864261	-0.098194
C	1.896118	1.272216	0.792767
C	1.908386	1.380474	-0.680948
C	2.592705	0.223874	-1.173418
C	2.985298	-0.583794	-0.077949
C	2.579727	0.047919	1.118617
C	1.747373	2.442202	1.745611
C	2.722790	-0.520789	2.504417
C	3.614638	-1.946733	-0.197073
C	2.733813	-0.170214	-2.616492
C	1.702046	2.658956	-1.464475
C	-1.951830	0.629691	2.755230
C	-3.698543	-1.528913	1.092891
C	-3.580396	-0.806767	-1.925138
C	-1.807423	1.869127	-2.302280
C	-1.416177	2.961152	0.693600
H	3.944314	-2.322776	0.783387
H	2.890789	-2.670699	-0.611058
H	4.488341	-1.929410	-0.871987
H	3.765630	-0.822978	2.701030
H	2.430051	0.212677	3.271157
H	2.089986	-1.416454	2.627898
H	1.217747	2.161260	2.669939
H	2.741985	2.826077	2.034008
H	1.195010	3.267332	1.278653
H	1.373050	2.452488	-2.494223
H	0.950636	3.310542	-0.999338
H	2.645563	3.231787	-1.520743

H	3.766153	-0.491713	-2.837887
H	2.069335	-1.022133	-2.847700
H	2.478006	0.657825	-3.294626
H	-2.504359	1.571214	-3.100416
H	-1.903674	2.960245	-2.159596
H	-0.784728	1.681532	-2.674438
H	-3.475019	-0.345164	-2.918284
H	-3.151545	-1.822901	-1.979969
H	-4.657824	-0.922557	-1.710423
H	-3.423822	-2.449027	0.549552
H	-3.495235	-1.691158	2.161887
H	-4.789809	-1.396788	0.971816
H	-2.238313	-0.313759	3.244599
H	-0.891008	0.817740	2.993923
H	-2.537504	1.443342	3.224006
H	-2.427606	3.401895	0.741261
H	-0.951553	3.076082	1.682615
H	-0.834539	3.548518	-0.031844

21-Pd

C 3.049680 -0.067703 1.548245
Si 1.969434 0.065506 -0.002517
C 3.046242 0.260964 -1.549713
Si -0.598738 -0.018827 -0.002716
N 0.634296 1.221943 0.126621
C 0.548765 2.691219 0.026240
C -0.625996 3.196128 0.892401
N 0.712283 -1.175506 -0.134118
C 0.725770 -2.646484 -0.024080
C -0.435672 -3.234419 -0.854729
C 2.068821 -3.183964 -0.564786
C 0.561904 -3.055309 1.459566
C 1.868301 3.312026 0.534256
C 0.316802 3.093224 -1.449857
H 0.572427 -4.153089 1.568961
H 1.380646 -2.633435 2.064637
H -0.394953 -2.670640 1.847854
H 2.087387 -4.284176 -0.511321
H 2.210371 -2.877846 -1.613166
H 2.913093 -2.800610 0.033807
H -0.457845 -4.332017 -0.755461
H -1.398772 -2.824736 -0.506680
H -0.314534 -2.972541 -1.917838
H 0.256069 4.189669 -1.555974
H 1.142129 2.722890 -2.079262
H -0.625145 2.649922 -1.811339
H -0.725364 4.290127 0.801830
H -1.568469 2.724221 0.567377
H -0.457906 2.937423 1.949887
H 1.813666 4.411483 0.492112
H 2.059721 3.007188 1.575214
H 2.718144 2.989793 -0.091626
H 3.714664 0.807037 1.651390
H 2.418188 -0.125514 2.449575
H 3.688179 -0.967705 1.519137
H 3.641535 1.189916 -1.513782

H 3.752029 -0.581050 -1.654149
H 2.416286 0.292642 -2.453408
Pd -2.743588 -0.090470 -0.000811

22-Pd
C 3.763610 -0.202778 1.871258
C 2.443983 -0.048035 1.420719
C 2.153494 -0.130594 0.045100
C 3.193106 -0.367440 -0.875167
C 4.512126 -0.511729 -0.422960
C 4.799190 -0.431083 0.950470
C 0.751140 0.025601 -0.425840
N -0.083159 -0.962966 -0.823208
C -0.045038 -2.402636 -0.457388
C 1.253336 -3.084344 -0.939897
N 0.049568 1.169408 -0.478406
Si -1.541531 0.239881 -0.869148
C 0.470407 2.582825 -0.380133
C 0.739340 2.956097 1.095918
C 1.721537 2.857193 -1.243203
C -0.714259 3.419924 -0.907817
C -0.203156 -2.549419 1.073537
C -1.252240 -3.054160 -1.164013
H -1.670700 0.501965 -2.348045
H 2.959222 -0.436506 -1.938562
H 5.314860 -0.690167 -1.141177
H 5.826523 -0.547661 1.301513
H 3.981680 -0.145644 2.939592
H 1.632191 0.126007 2.128200
H -0.485702 4.492101 -0.809053
H -0.904536 3.194364 -1.968785
H -1.625493 3.196105 -0.329101
H 1.940136 3.937189 -1.231566
H 2.600837 2.322288 -0.858559
H 1.541921 2.546878 -2.284821
H 0.940477 4.037126 1.173553
H -0.140907 2.713057 1.710932
H 1.611758 2.412057 1.484513
H -1.289689 -4.126773 -0.918309
H -2.189195 -2.579633 -0.825676
H -1.166477 -2.943228 -2.256762
H -0.286072 -3.614180 1.347547
H 0.668330 -2.122406 1.593579
H -1.113948 -2.014524 1.394311
H 1.158123 -4.172199 -0.792925
H 1.415248 -2.889362 -2.011894
H 2.130905 -2.737947 -0.378750
Pd -3.098965 0.008286 0.618611

23-Pd
C -3.917703 -0.205892 -1.807842
C -2.574088 -0.086399 -1.421641
C -2.229386 -0.098010 -0.056505
C -3.237852 -0.229850 0.917510
C -4.580345 -0.339861 0.528970
C -4.922047 -0.329107 -0.834082

C -0.802986 0.022176 0.353170
N 0.017029 -0.988520 0.716239
C -0.088666 -2.433100 0.400765
C -1.392466 -3.051292 0.949848
N -0.071178 1.146707 0.379842
Si 1.515492 0.172930 0.705310
C 1.846001 0.466502 2.568954
C -0.445447 2.564403 0.210162
C -0.724186 2.863160 -1.281124
C -1.671979 2.931959 1.073870
C 0.775300 3.387904 0.673770
C 0.010070 -2.634278 -1.129093
C 1.120526 -3.104118 1.086448
H -2.961876 -0.243839 1.973064
H -5.358509 -0.436589 1.288708
H -5.967680 -0.417986 -1.135805
H -4.178908 -0.202143 -2.867993
H -1.787561 0.008506 -2.171462
H 0.582355 4.459810 0.514291
H 0.972150 3.218170 1.743620
H 1.669674 3.097186 0.098421
H -1.851832 4.016937 1.004908
H -2.575963 2.409108 0.732632
H -1.486486 2.673611 2.128699
H -0.881592 3.945326 -1.420925
H 0.134273 2.543934 -1.891973
H -1.625406 2.334633 -1.622926
H 1.113026 -4.184965 0.877043
H 2.059673 -2.674287 0.698709
H 1.078412 -2.953457 2.177086
H 0.064501 -3.708981 -1.370047
H -0.873108 -2.209206 -1.630595
H 0.916313 -2.125055 -1.499481
H -1.347057 -4.145115 0.824596
H -1.503535 -2.826091 2.022555
H -2.277489 -2.681285 0.415725
H 2.424195 -0.377738 2.981963
H 2.449473 1.377562 2.717198
H 0.906361 0.562697 3.140558
Pd 2.966963 -0.072484 -0.884230

24-Pd
C 4.223456 -0.162279 -1.617283
C 2.850932 -0.088337 -1.337381
C 2.403281 -0.061362 -0.002454
C 3.339590 -0.105938 1.048580
C 4.711382 -0.169022 0.765559
C 5.155612 -0.198550 -0.567163
C 0.948360 0.037603 0.287618
N 0.180046 1.119692 0.109378
C 0.504175 2.529723 -0.178170
C 1.698303 3.020588 0.668097
N 0.131332 -0.958438 0.701991
Si -1.405500 0.094181 0.291751
N -2.094698 0.542936 1.823977
C -3.516613 0.823194 1.982319

C 0.330050 -2.425224 0.580002
C 0.513586 -2.813940 -0.904817
C 1.530180 -2.904663 1.424617
C -0.961394 -3.074628 1.121612
C -1.300487 0.872412 2.999106
C 0.794460 2.707152 -1.687014
C -0.755800 3.343431 0.193140
H 2.986324 -0.087602 2.080806
H 5.432709 -0.197335 1.584721
H 6.224092 -0.250568 -0.785977
H 4.563549 -0.190937 -2.654442
H 2.119871 -0.061111 -2.146148
H -0.869248 -4.170961 1.075638
H -1.136655 -2.772936 2.166166
H -1.825183 -2.762330 0.511880
H 1.545366 -4.006509 1.432413
H 2.485512 -2.551654 1.013984
H 1.433524 -2.549055 2.463013
H 0.535799 -3.911448 -1.009189
H -0.330329 -2.406288 -1.487463
H 1.456635 -2.407379 -1.300948
H -0.583488 4.408071 -0.028447
H -1.621689 2.994375 -0.391761
H -0.987178 3.231562 1.262904
H 0.887125 3.779465 -1.926631
H 1.733295 2.207373 -1.965961
H -0.031157 2.276706 -2.274787
H 1.833073 4.102223 0.507877
H 1.504213 2.846386 1.738566
H 2.630075 2.510804 0.388215
H -3.695918 1.898372 2.194426
H -4.047420 0.553447 1.054992
H -3.943404 0.239142 2.822492
H -1.346025 1.957751 3.232864
H -1.669989 0.325654 3.889738
H -0.248004 0.594459 2.838140
Pd -2.558471 -0.431054 -1.466896

25-Pd
C -5.585553 0.050722 0.157016
C -4.880731 -0.268134 -1.016157
C -3.478889 -0.251882 -1.020335
C -2.776204 0.069427 0.156636
C -3.482655 0.383333 1.332902
C -4.885152 0.379703 1.329574
C -1.289925 0.090655 0.152370
N -0.519786 1.024844 -0.431690
C -0.782235 2.462061 -0.672315
C 0.473042 3.016210 -1.378331
N -0.469361 -0.846311 0.670453
Si 1.034367 0.014027 -0.123569
O 1.725066 0.907938 1.127788
C 3.131987 0.936560 1.498527
C 3.958709 1.561184 0.359169
C -0.743812 -2.293077 0.878085
C 0.558546 -2.891556 1.449610

C -1.892589 -2.516957 1.884582
C -1.066077 -2.960741 -0.478262
C -2.014938 2.687330 -1.573797
C -0.971282 3.164975 0.691830
C 3.195595 1.813468 2.760272
C 3.630764 -0.488736 1.804199
H -2.928292 0.621678 2.241860
H -5.429994 0.628588 2.242400
H -6.677456 0.043293 0.157092
H -5.422534 -0.524040 -1.928899
H -2.920927 -0.480446 -1.929414
H 0.326421 4.083476 -1.605580
H 1.354784 2.909157 -0.729809
H 0.660386 2.469046 -2.315369
H -1.084668 4.251764 0.545486
H -1.875101 2.784061 1.193384
H -0.097173 2.972232 1.331079
H -2.078213 3.757966 -1.827051
H -1.917682 2.111284 -2.507201
H -2.947337 2.396821 -1.071986
H 0.424400 -3.970700 1.622242
H 1.386038 -2.743512 0.735453
H 0.819101 -2.406801 2.403740
H -1.172018 -4.050666 -0.348741
H -2.008040 -2.565692 -0.889996
H -0.246076 -2.751918 -1.186457
H -1.943646 -3.589657 2.131187
H -1.706654 -1.952729 2.812168
H -2.863747 -2.213082 1.472428
H 4.236496 1.900166 3.111459
H 2.810296 2.821862 2.540018
H 2.584347 1.369772 3.561999
H 4.677815 -0.460704 2.148247
H 3.010619 -0.947696 2.590549
H 3.568443 -1.107120 0.892667
H 5.022441 1.614335 0.644047
H 3.857384 0.945967 -0.550931
H 3.600223 2.580481 0.142657
Pd 2.109372 -1.062480 -1.662736

26-Pd
C -5.454711 -0.130443 0.095319
C -4.722210 -0.344598 -1.084661
C -3.322313 -0.270511 -1.066039
C -2.648393 0.002698 0.139666
C -3.382661 0.212000 1.322252
C -4.783613 0.151770 1.296869
C -1.163978 0.079752 0.157668
N -0.423720 1.068800 -0.374093
C -0.740221 2.507711 -0.534456
C 0.516615 3.161263 -1.146157
N -0.314022 -0.847605 0.642832
Si 1.165383 0.106039 -0.094377
O 1.824292 0.973713 1.193796
C 3.240042 0.933507 1.481439
C 3.529217 -0.206836 2.465551

C -0.535757 -2.312038 0.782387
C 0.780092 -2.886654 1.347027
C -1.689209 -2.624919 1.759623
C -0.815831 -2.930033 -0.606501
C -1.943551 2.734970 -1.474410
C -1.020142 3.112788 0.860629
C 3.637613 2.305150 2.036427
H -2.850619 0.413902 2.253032
H -5.349953 0.319876 2.215039
H -6.545237 -0.182630 0.078134
H -5.240881 -0.563797 -2.020094
H -2.744018 -0.418353 -1.979119
H 0.332165 4.235193 -1.303552
H 1.376400 3.042221 -0.470154
H 0.761859 2.691951 -2.111718
H -1.175479 4.200978 0.776479
H -1.927344 2.664450 1.296014
H -0.166905 2.918539 1.527145
H -2.045222 3.815061 -1.668119
H -1.782564 2.220170 -2.434354
H -2.881105 2.375157 -1.030273
H 0.687587 -3.977762 1.461841
H 1.612038 -2.669216 0.655387
H 1.005383 -2.441453 2.328847
H -0.889366 -4.027161 -0.524637
H -1.763912 -2.547236 -1.015825
H 0.006966 -2.667454 -1.293149
H -1.695709 -3.707504 1.964664
H -1.544075 -2.089247 2.711053
H -2.666233 -2.349163 1.341586
H 3.789508 0.737761 0.540020
H 4.717684 2.330378 2.255611
H 3.405991 3.096631 1.306368
H 3.084016 2.513358 2.967071
H 4.600630 -0.231004 2.726404
H 2.941610 -0.067581 3.388113
H 3.255781 -1.172162 2.011895
Pd 2.327382 -0.875217 -1.631734

27-Pd
C 4.809222 0.556217 1.880714
C 5.750619 0.390435 0.850580
C 5.317863 0.130564 -0.460349
C 3.946950 0.041385 -0.743699
C 3.002057 0.201315 0.287602
C 3.439020 0.455032 1.603076
C 1.545737 0.082705 0.017670
N 0.774800 0.965943 -0.632666
C 1.003377 2.402394 -0.921859
C 2.149312 2.587726 -1.941651
N 0.748723 -0.945848 0.401818
Si -0.752035 -0.143245 -0.432382
P -1.696320 0.862599 1.430266
C -2.341781 -0.688832 2.346131
C -3.327444 -1.568672 1.551525
C 1.150798 -2.382856 0.474165

C 2.203276 -2.629592 1.576697
C -0.115529 -3.200864 0.794858
C 1.685794 -2.822213 -0.908717
C -3.365631 1.636341 0.864369
C -3.348139 3.156961 1.137884
C -3.825990 1.348958 -0.577426
C -0.306656 2.923377 -1.546128
C 1.308494 3.172258 0.382267
C -2.952938 -0.269639 3.700593
H 2.698255 0.566409 2.396237
H 5.142075 0.759032 2.900614
H 6.817994 0.462825 1.069125
H 6.046724 -0.002612 -1.262272
H 3.601489 -0.155307 -1.759271
H 0.134696 -4.272781 0.770976
H -0.503387 -2.957820 1.794732
H -0.896245 -3.001126 0.041916
H 2.335261 -3.716238 1.703990
H 3.177917 -2.193730 1.321565
H 1.863160 -2.203467 2.533794
H 1.895099 -3.904490 -0.908270
H 0.923593 -2.596378 -1.674203
H 2.617053 -2.288821 -1.153990
H -0.193048 3.984581 -1.815537
H -0.559272 2.345572 -2.448904
H -1.137345 2.835339 -0.830796
H 2.185177 3.644137 -2.253250
H 3.122319 2.325769 -1.505683
H 1.972028 1.963910 -2.831748
H 1.394652 4.249161 0.163288
H 0.499498 3.014764 1.111709
H 2.257423 2.829404 0.820944
H -4.337078 3.593582 0.909973
H -3.101330 3.375691 2.189245
H -2.604418 3.668899 0.504870
H -4.823605 1.795581 -0.744509
H -3.132761 1.785966 -1.313464
H -3.874559 0.269874 -0.788025
H -4.107048 1.188508 1.548111
H -1.430210 -1.271079 2.555076
H -3.595668 -2.465620 2.138959
H -4.257547 -1.015543 1.343142
H -2.904591 -1.888269 0.585037
H -3.268581 -1.164252 4.266415
H -2.231906 0.297256 4.310984
H -3.846468 0.360576 3.553935
Pd -1.716112 -1.183294 -2.070418

28-Pd
C -4.234691 -0.809755 -0.125167
C -3.291813 0.236623 -0.094639
C -3.729726 1.572460 -0.174682
C -5.099427 1.857058 -0.283527
C -6.036516 0.811851 -0.321556
C -5.601355 -0.522027 -0.244307
C -1.841344 -0.068260 0.043209

N -0.917940 -0.078901 -0.947630
C -1.142068 -0.313681 -2.400162
C -1.887301 0.876569 -3.041011
N -1.209401 -0.430293 1.170664
Si 0.388528 -0.788974 0.229838
P 1.812018 0.829752 0.950464
Si 3.795388 0.061340 0.140617
C 5.073952 1.472920 0.318225
C -1.595800 -0.269008 2.591907
C -2.965783 -0.915139 2.897634
C -0.510246 -0.983893 3.423820
C -1.627346 1.235200 2.944725
Si 1.487674 2.823809 -0.085088
C 2.415395 4.124647 0.965238
C 2.162328 2.952139 -1.869781
C -0.371449 3.254573 -0.096066
C 0.253805 -0.450072 -3.039541
C -1.918746 -1.632176 -2.618150
C 4.301594 -1.418376 1.225370
C 3.715036 -0.516926 -1.672972
H -2.996578 2.378954 -0.151666
H -5.432835 2.895287 -0.339923
H -7.101742 1.034974 -0.409739
H -6.326165 -1.338150 -0.271830
H -3.889870 -1.841543 -0.048619
H 0.152541 -0.551477 -4.131088
H 0.870625 0.431878 -2.817992
H 0.765841 -1.339230 -2.637513
H -1.967984 0.707906 -4.126995
H -2.900800 0.987169 -2.632250
H -1.331072 1.812484 -2.874871
H -1.941470 -1.878398 -3.692418
H -1.408748 -2.443950 -2.072992
H -2.955262 -1.546035 -2.261810
H -0.766718 -0.914546 4.492395
H -0.446716 -2.044400 3.134719
H 0.473257 -0.517070 3.265218
H -3.119707 -0.912751 3.988691
H -3.793826 -0.364058 2.433349
H -2.985063 -1.957673 2.544169
H -1.871522 1.364391 4.011837
H -0.644531 1.688832 2.747718
H -2.392686 1.753391 2.345881
H 6.071699 1.126980 -0.005803
H 4.808857 2.350690 -0.293824
H 5.156034 1.807223 1.366168
H 5.242401 -1.872180 0.865140
H 4.438374 -1.124794 2.279730
H 3.505970 -2.185710 1.181853
H 4.704812 -0.869087 -2.016469
H 3.003577 -1.359587 -1.740899
H 3.374677 0.275906 -2.357844
H 2.293933 5.133213 0.530138
H 2.031293 4.149154 1.998745
H 3.494666 3.905141 1.015229
H -0.522995 4.301255 -0.414659

H -0.908299 2.594933 -0.793697
H -0.818243 3.131294 0.903411
H 2.153401 4.007481 -2.197782
H 3.200628 2.589586 -1.933417
H 1.560434 2.374468 -2.588568
Pd 1.111253 -2.803015 -0.145141

29-Pd
C 5.048580 -0.322460 -0.701360
C 4.096063 -0.235299 -1.729772
C 2.733175 -0.117238 -1.418453
C 2.319054 -0.095403 -0.073278
C 3.274288 -0.190985 0.957029
C 4.636182 -0.298266 0.641623
C 0.875360 0.023897 0.266089
N 0.053498 -0.980248 0.640949
C 0.186208 -2.440654 0.401378
C -1.073686 -3.086544 1.015616
N 0.132674 1.141062 0.214819
Si -1.446137 0.153265 0.464495
Cl -1.930030 0.576410 2.508531
C 0.501175 2.563305 0.035611
C -0.772332 3.381605 0.335334
C 1.620613 2.966125 1.019810
C 0.940700 2.820655 -1.423960
C 0.220268 -2.717586 -1.119128
C 1.442221 -3.014445 1.090885
H 2.942790 -0.179714 1.996332
H 5.373793 -0.366355 1.443552
H 6.109201 -0.409874 -0.945273
H 4.412631 -0.257574 -2.774366
H 1.987004 -0.046699 -2.210873
H -1.035253 -4.177016 0.869726
H -1.132704 -2.870069 2.093342
H -1.980068 -2.694840 0.523786
H 1.419100 -4.113078 1.010879
H 2.367099 -2.655369 0.620423
H 1.452892 -2.740833 2.157515
H 0.200092 -3.803852 -1.305556
H -0.658654 -2.249908 -1.593937
H 1.136437 -2.304675 -1.568538
H -0.564486 4.451051 0.179262
H -1.590235 3.076951 -0.337767
H -1.097154 3.227023 1.374691
H 1.080289 3.902760 -1.580094
H 1.890358 2.314357 -1.647018
H 0.166020 2.458416 -2.117653
H 1.815506 4.046265 0.923358
H 1.311432 2.755191 2.055271
H 2.553800 2.426014 0.806463
Pd -2.884650 -0.179973 -1.106444

30-Pd
C -5.303612 -0.334226 -0.282739
C -4.493263 -0.539199 -1.411868
C -3.100183 -0.411193 -1.310406

C -2.513553 -0.087567 -0.072535
C -3.325714 0.112560 1.060115
C -4.718782 -0.004713 0.951406
C -1.035995 0.021248 0.054749
N -0.270196 1.054847 -0.335760
C -0.624187 2.458816 -0.652096
C 0.705789 3.187286 -0.935665
N -0.210008 -0.916134 0.562654
Si 1.300074 0.090261 0.039271
Br 1.934243 1.033549 2.071173
C -0.397376 -2.387493 0.650748
C 0.873008 -2.934896 1.334338
C -1.634709 -2.756199 1.496144
C -0.511795 -2.971502 -0.775823
C -1.521556 2.531053 -1.907447
C -1.331133 3.108004 0.558770
H -2.859611 0.352079 2.017046
H -5.345729 0.155172 1.830715
H -6.388041 -0.431171 -0.364343
H -4.944958 -0.795965 -2.372024
H -2.463502 -0.559004 -2.183774
H 0.497512 4.232097 -1.212347
H 1.351209 3.179656 -0.044539
H 1.242335 2.697838 -1.763964
H -1.532824 4.169462 0.341752
H -2.289335 2.607990 0.764950
H -0.690707 3.042376 1.451207
H -1.663571 3.587054 -2.187900
H -1.041985 2.005213 -2.747828
H -2.509191 2.087652 -1.723056
H 0.798359 -4.029492 1.425533
H 1.763729 -2.689359 0.731581
H 0.991814 -2.497280 2.337372
H -0.545582 -4.072422 -0.732749
H -1.429486 -2.612571 -1.267432
H 0.363652 -2.655429 -1.368112
H -1.636164 -3.845504 1.660544
H -1.594383 -2.253902 2.475283
H -2.572133 -2.483262 0.993770
Pd 2.686062 -0.685912 -1.418194

31-Pd

C	3.066877	-1.738877	-0.612272
C	2.651739	-0.661635	0.211809
C	3.589235	0.079754	0.984962
C	4.938795	-0.309801	0.953457
C	5.361193	-1.392357	0.169512
C	4.431966	-2.086635	-0.611485
N	1.267264	-0.322503	0.341691
Si	-0.137188	0.404311	-0.828042
N	-0.507992	2.065781	-0.319876
Si	0.784220	3.285386	-0.524493
C	2.344184	2.518170	-1.300546
C	3.141248	1.266236	1.840599
C	4.146424	2.436637	1.798868
C	2.106918	-2.533302	-1.493021

C	2.064038	-4.024929	-1.095176
C	0.367003	-1.192705	0.869684
N	0.610134	-2.312824	1.608740
C	1.824361	-2.545401	2.393880
N	-0.853733	-0.812951	0.432660
C	-2.094916	-1.122911	1.045251
C	-2.369320	-0.637742	2.350188
C	-3.615881	-0.947518	2.922817
C	-4.577236	-1.679141	2.213203
C	-4.290709	-2.134826	0.919807
C	-3.045062	-1.883891	0.318078
C	-1.366644	0.214004	3.129028
C	-0.778996	-0.584997	4.314895
C	-2.734133	-2.442847	-1.070422
C	-3.476693	-1.667930	-2.182959
C	-0.348517	-3.425690	1.622664
C	-3.053127	-3.953726	-1.161754
C	-1.988129	1.538493	3.625887
Si	-2.171422	2.690968	-0.567078
C	-2.490480	3.017332	-2.417899
C	-3.551440	1.510713	-0.018640
C	-2.407502	4.267030	0.485683
C	2.851431	0.868190	3.307298
C	2.474421	-2.372375	-2.984601
C	0.356851	4.668634	-1.772127
C	1.116632	4.134675	1.152608
H	-5.040084	-2.706513	0.368698
H	-5.547813	-1.892405	2.666745
H	-3.841009	-0.588487	3.929178
H	4.763003	-2.917066	-1.238871
H	5.668937	0.241760	1.547748
H	-1.659321	-2.300246	-1.267431
H	-3.334786	-2.178186	-3.150665
H	-4.558309	-1.607041	-1.973614
H	-3.061957	-0.652544	-2.280959
H	-2.713987	-4.346463	-2.134165
H	-2.555118	-4.525544	-0.361414
H	-4.136759	-4.140125	-1.083129
H	-0.543677	0.490883	2.457209
H	-0.021429	0.014714	4.846352
H	-1.573297	-0.850895	5.032209
H	-0.306138	-1.514986	3.965097
H	-1.219263	2.140560	4.137936
H	-2.382710	2.123370	2.782603
H	-2.808894	1.357511	4.338889
H	1.093806	-2.119561	-1.392247
H	1.760614	-2.939278	-3.605551
H	2.412088	-1.309778	-3.271080
H	3.491867	-2.745168	-3.192042
H	1.333601	-4.560869	-1.723875
H	3.047795	-4.504225	-1.232293
H	1.768428	-4.145548	-0.042099
H	2.194909	1.622620	1.419925
H	3.706887	3.314611	2.296347
H	5.081927	2.185750	2.325559
H	4.393225	2.708533	0.762017

H	2.632723	1.770673	3.902772
H	1.977253	0.204543	3.378933
H	3.720552	0.361166	3.759344
H	1.528739	-2.878356	3.403358
H	2.447582	-3.323834	1.922938
H	2.414488	-1.634072	2.482777
H	0.224486	-4.360658	1.723030
H	-1.064045	-3.344754	2.457545
H	-0.900682	-3.457250	0.678534
H	1.194445	5.389876	-1.780873
H	0.263289	4.254832	-2.789396
H	-0.562426	5.228971	-1.550916
H	2.043951	4.732573	1.118220
H	0.286850	4.816864	1.401958
H	1.207551	3.413239	1.979557
H	3.100739	3.313087	-1.428927
H	2.814910	1.697540	-0.749291
H	2.085173	2.131139	-2.301419
H	-3.573580	3.073567	-2.627153
H	-2.021281	3.939166	-2.793540
H	-2.071627	2.167550	-2.989579
H	-3.445360	4.626655	0.368229
H	-2.251498	4.046901	1.555324
H	-1.737133	5.096980	0.217359
H	-4.504024	2.022780	-0.248040
H	-3.554972	0.560003	-0.566926
H	-3.548685	1.275173	1.054133
H	6.414229	-1.682712	0.158397
Pd	-0.231948	-0.213753	-2.906239

32-Pd

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C -4.818907 -0.653925 -0.975296
C -5.933388 -1.469075 -1.220669
C -5.947928 -2.798244 -0.765880
C -4.843203 -3.310357 -0.065557
C -2.515791 -0.302460 -0.050461
N -2.384674 0.667421 0.870700
C -3.163083 0.930631 2.099596
C -4.628472 1.290343 1.765489
N -1.370670 -0.307152 -0.769850
C -1.143272 -0.756247 -2.161723
C -1.450288 -2.258925 -2.339382
Si -0.711213 1.209524 0.160750
Si 0.913315 0.523572 1.807421
N 2.495490 0.883458 0.809115
C 3.244010 2.078150 0.362107
C 2.591156 3.292643 1.052200
N 1.592902 -1.065468 0.973023
C 1.400453 -2.498870 1.271832
C 2.247672 -2.913041 2.497669
C 2.695927 -0.417416 0.532719
C 3.919710 -1.036204 -0.050784
C 4.003790 -1.297824 -1.431939
C 5.153581 -1.896247 -1.968754

C 6.226661 -2.240157 -1.130517
C 6.149129 -1.978920 0.247809
C 5.002085 -1.377003 0.784944
C -0.099359 -2.656500 1.601856
C 1.745583 -3.397808 0.063528
C 4.733221 2.000274 0.771532
C 3.111944 2.228181 -1.170048
C -1.999566 0.091640 -3.129821
C 0.352100 -0.495989 -2.444418
C -3.110593 -0.301981 3.029959
C -2.493281 2.136485 2.790932
H -2.859946 -2.894267 0.709331
H -4.851169 -4.342031 0.292311
H -6.817040 -3.431574 -0.955573
H -6.790062 -1.065980 -1.764794
H -4.803394 0.382136 -1.316089
H -3.067009 2.411400 3.689697
H -1.463650 1.887973 3.094082
H -2.460229 2.997465 2.104741
H -3.640154 -0.084314 3.971700
H -3.589614 -1.169520 2.551519
H -2.063989 -0.551626 3.263287
H -5.139489 1.616638 2.685936
H -4.657468 2.113685 1.034970
H -5.172318 0.428366 1.356366
H 0.610569 -0.851993 -3.454263
H 0.556919 0.585729 -2.379343
H 0.971824 -1.017522 -1.700326
H -1.747922 -0.153612 -4.175188
H -3.070870 -0.107005 -2.973386
H -1.795691 1.159945 -2.941982
H -1.128686 -2.573446 -3.345413
H -0.904417 -2.858231 -1.594415
H -2.523833 -2.467608 -2.241316
H 3.636388 3.140135 -1.500395
H 3.556981 1.363560 -1.685761
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H 1.448628 -4.433905 0.293693
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H 2.820921 -3.389621 -0.156463
H 2.015763 -3.951671 2.786983
H 3.320791 -2.849776 2.263741
H 2.025994 -2.247725 3.346848
H 4.941408 -1.157700 1.851963
H 6.982387 -2.240282 0.903533
H 7.120270 -2.707783 -1.549193
H 5.210383 -2.094471 -3.041161

H 3.164288 -1.036989 -2.076906
Pd -0.596765 3.047691 -1.006751

33-Pd
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C -4.161565 1.064750 0.362794
C -5.202534 0.985387 -0.595994
C -6.434179 1.597679 -0.353241
C -6.678488 2.308119 0.840955
C -5.642174 2.377834 1.794117
C -2.870252 0.425399 0.136100
N -2.325946 0.049801 -1.040404
C -2.715765 0.363081 -2.370613
C -3.285568 -0.668219 -3.161327
C -3.656297 -0.358636 -4.481927
C -3.473566 0.928014 -5.005082
C -2.895850 1.926356 -4.210550
C -2.495477 1.662797 -2.888762
C -3.521395 -2.074325 -2.614617
C -5.016327 -2.461626 -2.669602
C -1.840278 2.760132 -2.057199
C -0.586489 3.330422 -2.759484
C -8.008462 2.991567 1.080857
N -1.954434 0.055503 1.088152
C -2.288364 -0.358827 2.418394
C -3.123404 -1.493815 2.620416
C -3.390162 -1.900559 3.939706
C -2.845399 -1.225943 5.037930
C -2.025601 -0.113915 4.822003
C -1.736142 0.340886 3.521914
C -3.759308 -2.281989 1.476482
C -3.385690 -3.778925 1.532905
C -0.849153 1.574948 3.360805
C -1.479153 2.809572 4.049377
Si -0.864865 -0.775308 -0.231001
Si 1.008888 0.130045 -1.348921
N 2.301751 -0.862315 -0.376099
C 2.543528 -2.227027 -0.067304
C 2.920215 -3.100109 -1.123312
C 3.138087 -4.456929 -0.824828
C 3.001113 -4.944022 0.481196
C 2.616831 -4.071506 1.506610
C 2.363651 -2.711080 1.255674
C 3.047146 -2.615992 -2.564345
C 4.400551 -2.998420 -3.202646
C 1.888762 -1.819323 2.395190
C 0.622454 -2.394921 3.068220
N 2.165234 1.295624 -0.312319
C 2.950595 0.237943 0.051841
C 4.257588 0.308594 0.700483
C 4.572625 1.406029 1.531755
C 5.815857 1.476543 2.168571
C 6.779413 0.462786 2.001370
C 6.459334 -0.629653 1.165628
C 5.222336 -0.712340 0.523684
C 8.123664 0.533574 2.696245

C 2.687168 2.579599 -0.683656
C 2.240648 3.733177 0.011176
C 2.664517 4.998218 -0.436172
C 3.529698 5.131197 -1.527051
C 3.986435 3.983689 -2.184377
C 3.576236 2.697770 -1.789161
C 1.329840 3.650307 1.234184
C 1.951621 4.383390 2.446403
C 4.112126 1.498733 -2.573327
C 3.691541 1.562358 -4.059166
C 5.649054 1.390996 -2.436930
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C 3.008284 -1.599494 3.439656
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C 0.560035 1.316496 3.941047
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H 4.996424 -1.562401 -0.118474
H 7.195241 -1.423925 1.015753
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H 3.835265 2.193116 1.679270
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H -8.020633 4.001901 0.633071
H -8.836703 2.423451 0.627500
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H -2.739292 2.926341 -4.619870
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H 6.143106 2.271874 -2.879364
H 5.946470 1.318909 -1.380411
H 1.205665 2.591276 1.499356
H 1.280083 4.317601 3.316986
H 2.924537 3.947303 2.725570
H 2.110036 5.450957 2.225897
H -0.719191 4.181691 1.803444

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H 1.619522 -0.843343 1.967059
H 0.235478 -1.694632 3.823687
H -0.162230 -2.565042 2.313310
H 0.843762 -3.352699 3.567268
H 2.652619 -0.931032 4.240825
H 3.290511 -2.561690 3.898956
H 3.905187 -1.156798 2.982965
H 2.983511 -1.519331 -2.571243
H 4.459583 -2.591363 -4.225631
H 5.242931 -2.592567 -2.617947
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H 1.881217 -4.248115 -3.449188
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H -1.578369 -2.886123 -3.171274
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H -5.631729 -1.751560 -2.093326
H -5.389951 -2.476331 -3.707119
H -1.508514 2.310805 -1.110199
H -2.371636 4.644030 -1.083972
H -3.192320 4.376108 -2.647377
H -3.728416 3.481358 -1.196798
H -0.087152 4.068048 -2.111796
H 0.131466 2.525523 -2.984461
H -0.856815 3.829548 -3.704584
H -3.365613 -1.915889 0.522143
H -3.833358 -4.303678 0.672706
H -2.289993 -3.894523 1.477043
H -3.751924 -4.256214 2.457033
H -5.732624 -2.621276 0.602505
H -5.740067 -2.517976 2.385938
H -5.567202 -1.033437 1.408291
H -0.746086 1.791896 2.288401
H 1.193844 2.208118 3.831445
H 0.499316 1.069281 5.013637
H 1.047536 0.480254 3.427274
H -0.809278 3.679534 3.958530
H -2.448422 3.076643 3.599505
H -1.642038 2.618115 5.122261
Pd -0.521883 -2.923861 -0.424080

34-Pd
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C 4.753439 -1.007853 1.189602
C 5.993486 -1.522994 0.762937
C 6.961549 -1.897237 1.706338
C 6.701831 -1.747391 3.078583
C 5.467839 -1.229316 3.506088
C 3.731255 -0.626979 0.179584
N 3.806872 0.412337 -0.670707
C 4.573865 1.678616 -0.563523

C 6.068270 1.434017 -0.870064
N 2.591650 -1.297862 -0.113525
C 2.326757 -2.755726 0.063224
C 2.304635 -3.156086 1.553304
Si 2.289211 -0.186352 -1.611086
C 0.999664 1.136755 -1.028695
C -0.454255 0.745022 -0.831245
C -0.973708 -0.336411 -1.582241
C -2.141448 -1.064970 -1.284898
C -2.289896 -2.438730 -1.912184
N -3.092231 -0.623759 -0.440752
Ge -3.259547 1.398934 -0.110438
N -1.204844 1.446476 0.038941
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C 0.052599 4.871679 0.860390
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C 0.976050 0.246159 2.725464
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C -4.722367 -3.234174 1.681546
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C -0.845232 1.114804 4.263898
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C 3.387042 -3.572444 -0.708381
C 3.995285 2.641184 -1.623499
C 4.399731 2.301622 0.840429
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H 5.261885 -1.111448 4.571780
H 7.457821 -2.034703 3.812160
H 7.916893 -2.304347 1.369372
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H 4.384504 -3.437414 -0.263472

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H 6.597261 2.400140 -0.902300
H 6.535201 0.809872 -0.096525
H 6.176332 0.937857 -1.847113
H 4.904608 3.280448 0.869859
H 3.332613 2.453589 1.066873
H 4.841386 1.660104 1.616053
H 1.019217 1.923757 -1.803829
H 1.375005 1.613962 -0.111481
H -0.303121 -0.772982 -2.323262
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H 0.926191 5.529949 2.728958
H 0.660267 3.316016 3.829948
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H -0.229130 4.776639 -3.221581
H 0.388399 5.694418 -1.825404
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H -2.597751 5.112875 -2.333242
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H -2.014297 5.935164 -0.855143
H -1.117017 0.414667 2.254534
H 0.903239 -0.717012 3.258927
H 1.268032 0.040036 1.685369
H 1.773164 0.843561 3.201583
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H -0.092887 1.610631 4.899829
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H -1.717998 -4.273102 0.617297
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H -2.721885 -0.982236 3.301240
H -2.930114 -2.675621 3.829855
H -1.621340 -2.534624 -2.779175
H -2.022486 -3.221820 -1.186741
H -3.331599 -2.619890 -2.217777
Pd 2.320746 -1.100575 -3.572740

35-Pd
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C -3.882983 0.907284 -0.190720
C -5.123626 1.068625 0.454666

C -6.170083 1.747399 -0.188153
C -5.983809 2.267036 -1.479601
C -4.746907 2.106677 -2.126436
C -2.770491 0.178002 0.487570
N -1.811492 0.717188 1.262882
C -1.661775 2.089698 1.779455
C -0.300976 2.109242 2.511776
Si -1.446520 -1.020828 2.074139
O 0.078468 -1.432547 1.465725
Si 1.266871 -1.466841 0.304736
N 1.111740 0.109284 -0.771015
C 0.755520 0.213097 -2.212270
C 1.930768 -0.265524 -3.095200
C 2.195390 0.639869 -0.155750
N 2.493987 -0.148924 0.882686
C 3.463739 -0.020494 1.989153
C 3.601354 1.433963 2.488148
C 2.951970 1.848116 -0.578648
C 4.233897 1.722099 -1.146905
C 4.951286 2.868019 -1.520614
C 4.397388 4.143135 -1.317880
C 3.119043 4.270292 -0.748512
C 2.394982 3.126603 -0.384259
C 2.927151 -0.904163 3.137065
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C 0.337157 1.645682 -2.604677
C -3.808358 -2.023949 -1.512192
C -2.498859 -3.512233 0.038539
C -1.626354 3.134270 0.643453
C -2.791846 2.430360 2.779553
H 1.402941 3.214237 0.059929
H 2.685579 5.259708 -0.589024
H 4.959455 5.034606 -1.603663
H 5.941504 2.765086 -1.968973
H 4.653635 0.727769 -1.302932
H 3.630492 -0.870833 3.983660
H 1.939777 -0.552607 3.469601
H 2.827460 -1.948625 2.801955
H 4.239226 1.438012 3.386346
H 4.063917 2.085626 1.735122
H 2.616465 1.844559 2.757925
H 5.526816 -0.624168 2.375874
H 4.701034 -1.571987 1.091288
H 5.272965 0.093505 0.758801
H -0.826046 -0.646707 -3.441170
H -0.142594 -1.773230 -2.221441
H -1.249302 -0.472206 -1.704256
H 1.615429 -0.307804 -4.151133
H 2.787258 0.421198 -3.015641
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H -0.007280 1.639653 -3.651775
H -0.490643 1.992721 -1.968416

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H -4.321786 -2.927439 -1.878548
H -4.495196 -1.173645 -1.616149
H -2.923916 -1.849549 -2.141317
H -5.214794 -3.361258 0.473795
H -4.380380 -2.621309 1.876684
H -5.332408 -1.600080 0.753252
H -3.039461 -4.384793 -0.360849
H -1.570831 -3.365094 -0.535394
H -2.222868 -3.722499 1.084414
H -0.098221 3.117943 2.905107
H -0.304478 1.399495 3.354897
H 0.503144 1.818158 1.820781
H -1.391776 4.123639 1.069459
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H -3.765140 2.459835 2.267717
H -2.828626 1.669430 3.574650
H -5.262263 0.663266 1.458175
H -7.129304 1.869323 0.319323
H -6.798948 2.793623 -1.980128
H -4.597577 2.507271 -3.131295
H -2.738371 1.298008 -1.984094
Pd 1.972891 -3.243022 -0.718893

36-Pd
C 6.213631 -0.608834 -1.231059
C 5.248293 -1.545163 -0.813873
C 5.411158 -2.907464 -1.126843
C 6.530793 -3.329150 -1.859535
C 7.495322 -2.394452 -2.271613
C 7.336998 -1.034981 -1.953137
C 4.050823 -1.080880 -0.062914
N 3.826925 -1.245262 1.251029
C 4.767962 -1.495247 2.364907
C 5.341253 -2.928488 2.296908
N 2.976795 -0.452619 -0.584828
C 2.446924 -0.533340 -1.972909
C 3.504524 -0.172138 -3.039379
Si 2.040798 -0.634664 1.084032
O 2.308149 0.948254 1.801715
C 1.411027 1.879371 1.299546
C 0.052738 1.605724 1.536256
C -0.944760 2.090597 0.686580
C -0.655484 3.170938 -0.186748
C 0.686542 3.601222 -0.197514
C 1.766626 2.958049 0.458426
O -2.154801 1.422236 0.675842
Si -2.161975 -0.325202 0.538102
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C -5.432814 1.164835 2.164486
C 3.190880 3.515610 0.227389
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C -1.737745 3.821303 -1.071614

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C -6.688989 -0.331309 -0.954761
C -8.005226 -0.732217 -1.227559
C -8.434949 -2.021999 -0.874374
C -7.547987 -2.908513 -0.240262
C -6.236385 -2.505155 0.046988
C -1.820489 -0.901147 -2.704865
C -3.401328 -2.761194 -2.114305
C -5.502604 -1.221604 3.026661
C -3.493784 0.224178 3.479879
C 1.913523 -1.961370 -2.235283
C 1.285612 0.479259 -2.043003
C -2.921333 4.301517 -0.190714
C -1.204973 5.046586 -1.850023
C 3.240486 4.956488 0.806154
C 4.320560 2.700977 0.899854
C 5.909682 -0.454133 2.342621
C 3.952052 -1.330229 3.664841
H 6.072723 0.445481 -0.988126
H 8.085440 -0.306366 -2.271116
H 8.367775 -2.724546 -2.839272
H 6.650403 -4.385935 -2.106978
H 4.659253 -3.625953 -0.796779
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H 5.490924 0.562332 2.369804
H 5.947074 -3.122810 3.197107
H 4.521310 -3.663024 2.258959
H 5.981388 -3.061317 1.413780
H 0.800518 0.413035 -3.028773
H 0.537235 0.252984 -1.266715
H 1.643138 1.504387 -1.882785
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H 2.734812 -2.694091 -2.175032
H 1.145932 -2.217129 -1.485843
H 2.993221 -0.061437 -4.009073
H 4.000024 0.779948 -2.798228
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H -0.196790 0.846431 2.274108
H 0.937429 4.457108 -0.820498
H 4.238781 5.397105 0.638726
H 2.490098 5.605889 0.328430
H 3.040858 4.940961 1.889766
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H 3.537190 2.560098 -1.710483
H 2.785946 4.171615 -1.850953
H 5.281951 3.207107 0.701886
H 4.178035 2.630227 1.986978

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H -0.816949 5.819965 -1.167280
H -0.400766 4.762638 -2.548639
H -3.701075 4.755937 -0.826674
H -3.362695 3.461603 0.362336
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H -1.430417 2.457548 -2.759208
H -2.703399 1.922591 -1.622451
H -5.543006 -3.181765 0.548214
H -7.878596 -3.912486 0.033484
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H -2.864793 1.048760 3.115145
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37-Pd
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C -5.624579 -0.851378 -1.637132
C -6.950036 -1.143100 -1.994312
C -7.995930 -0.888169 -1.092891
C -7.712347 -0.337154 0.168026
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N -3.010418 -0.842279 0.513904
C -3.210214 -2.216238 1.028781
C -4.333420 -2.285519 2.090541
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N -3.347380 1.229146 0.008925
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C -4.224624 2.420332 -1.986019
P -0.200818 0.728358 -0.480246
Si -0.193542 -0.749264 -2.171726
C -1.917431 -0.742721 -2.992534
Si 1.605306 0.548651 0.842476
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C 3.614652 -0.050249 -0.230192
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C 7.437466 -1.135767 -1.871564
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H 1.100942 -3.007946 0.897185
H 1.473793 3.030453 -1.407371
H 2.601585 4.399752 -1.129031
H 1.897741 3.507604 0.256109
H 3.185902 -3.417855 -0.610027
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H 4.083023 -1.379632 -2.516727
H 8.294976 -0.189951 -0.117644
H 4.288227 3.104744 1.133385
H 4.860648 4.070527 -0.263923
H 5.535109 2.444697 0.025695
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H -1.671166 -1.987763 2.568207
H 4.963787 -1.341906 1.972358
H 4.168995 -2.574213 2.991807
H 3.492383 -0.907402 2.910257
H 4.899245 1.676901 -2.307908
H 4.220375 3.287111 -2.661197
H 3.207198 1.829742 -2.870855
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H 0.274493 -3.173210 -2.651146
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H -2.663510 -1.081593 -2.257562
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38-Pd
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C 1.636798 2.648806 2.724416
C 0.862668 3.435901 1.805478
Si 1.832712 0.151950 -0.642812
N 3.612068 0.663594 -1.141066
C 4.233424 1.917486 -1.618234
C 5.416054 1.655734 -2.577521
Fe -0.003382 1.605756 2.083164
C -2.047910 1.597853 1.914952
C -1.530030 0.286891 1.594479
C -0.791663 -0.146487 2.762059
C -0.876986 0.867513 3.777267
C -1.651552 1.954250 3.247028
Si -1.821114 -0.643605 -0.040414
N -3.585457 -1.299592 0.320569
C -4.182188 -2.117271 1.397545
C -3.061017 -3.045383 1.911384
C 4.145910 -0.332337 -0.415392
N 3.132638 -0.931222 0.248096
C 3.051878 -2.332853 0.726771
C 1.775083 -2.422557 1.585966
C 5.577941 -0.734075 -0.413608
C 6.411785 -0.389055 0.667080
C 7.763410 -0.761860 0.659331
C 8.286669 -1.489747 -0.422584
C 7.455621 -1.838917 -1.500809
C 6.106273 -1.457566 -1.500123
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C 4.705196 2.750788 -0.402241
C 3.131678 2.687339 -2.376198

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C -7.771491 0.787484 -0.483428
C -8.302971 -0.054816 -1.474632
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C -3.088497 1.334469 -2.042318
C -2.966043 0.432107 -3.291032
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C -4.313041 2.267459 -2.178117
C -4.651997 -1.186892 2.540503
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H 5.992561 0.165572 1.508264
H 8.406952 -0.487964 1.497962
H 9.338346 -1.783803 -0.425745
H 7.859193 -2.405327 -2.342778
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39-Pd
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C 5.225676 -1.443834 0.306242
C 6.051773 -2.187352 -0.553441
C 5.538832 -2.672282 -1.766438
C 4.200009 -2.410518 -2.111395
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C -0.019101 -2.213327 2.304348
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N 2.544209 0.950359 0.313359
C 3.428351 2.088484 0.014277
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Si -0.952076 1.347962 -0.130886
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C -5.395769 -2.464532 -1.475625
C -5.308969 -3.624746 -0.688481
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C -3.316016 -2.744062 0.393696
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C -4.459523 1.551288 0.936944
C 0.346452 -0.051291 -2.755489
C -0.257991 -2.244293 -1.634455
C 4.130897 1.873847 -1.348904
C 2.546919 3.352806 -0.061938
C 2.283761 -3.158752 1.944111
C 1.918557 -1.347190 3.666713
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H -4.519750 -1.007191 1.948422
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H -0.048327 0.889844 -3.169426
H 1.062567 0.194383 -1.955376
H -1.242079 -1.670544 -4.216519
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H -2.253126 -0.277373 -3.728374
H 0.318210 -2.787442 -2.401141
H 0.397698 -2.024666 -0.778293
H -1.084709 -2.890289 -1.300828
H 4.763103 2.744871 -1.591224
H 4.765113 0.976180 -1.327278
H 3.377895 1.748996 -2.142514
H 5.101500 3.174197 0.911129
H 4.011311 2.398106 2.102750
H 5.170767 1.409695 1.161746
H 3.154595 4.219777 -0.366815
H 1.726705 3.218338 -0.788224
H 2.094738 3.571941 0.920023
H -0.234097 -2.933968 3.109975
H -0.624699 -1.307287 2.476552
H -0.321209 -2.650896 1.341149
H 2.077679 -3.933680 2.700676
H 2.000725 -3.538535 0.950734
H 3.365389 -2.958737 1.935313
H 1.746575 -2.112977 4.441470
H 2.990359 -1.092225 3.675059
H 1.346126 -0.443753 3.930240
H 0.816714 1.435975 2.422736
H 5.618252 -1.064743 1.254468
H 7.089589 -2.387242 -0.276704
H 6.175895 -3.251073 -2.439232
H 3.795837 -2.787655 -3.054271
H 2.349892 -1.455809 -1.509244
H 3.608744 -0.160689 1.823485
Pd -1.191637 3.413015 -0.732194

40-Pd
C 2.947237 2.972609 0.434110
C 3.234730 1.821635 -0.324867
C 4.385667 1.789515 -1.136422
C 5.245842 2.896407 -1.180616
C 4.955946 4.043612 -0.423766
C 3.804443 4.080908 0.380037
C 2.338406 0.635602 -0.273196
N 2.304218 -0.315950 0.687247
C 3.362520 -0.708965 1.653541
C 4.586886 -1.243239 0.875937

N 1.434481 0.274223 -1.201750
C 0.802212 1.054716 -2.289077
C 0.124774 2.309496 -1.696034
Si 1.067834 -1.333766 -0.307265
Si -0.959035 -0.877934 0.800363
Cl -0.967272 -2.172234 2.538496
N -1.642949 0.698261 1.169213
C -1.462709 1.667312 2.263620
C -2.450436 1.408505 3.426979
C -2.987276 0.244508 0.692111
N -2.483376 -0.935847 -0.064843
C -3.359597 -2.034101 -0.513043
C -2.445170 -3.203088 -0.936568
C -3.770139 1.276409 -0.102596
C -3.332170 1.722647 -1.361347
C -4.044915 2.709634 -2.052695
C -5.212153 3.262093 -1.493918
C -5.664817 2.812203 -0.244047
C -4.945554 1.820340 0.443546
C -0.017539 1.504842 2.780879
C -1.653704 3.109672 1.735176
C -4.304432 -2.505940 0.619332
C -4.201057 -1.577629 -1.727204
C 1.841295 1.447499 -3.361902
C -0.250138 0.120935 -2.922979
C 3.767073 0.468175 2.566753
C 2.762560 -1.838990 2.513010
H 2.056900 2.993272 1.062927
H 3.574049 4.971717 0.967629
H 5.624576 4.905977 -0.461099
H 6.139083 2.863373 -1.807517
H 4.596840 0.898521 -1.729260
H 3.522388 -2.202266 3.222038
H 1.889325 -1.480461 3.077130
H 2.443883 -2.678674 1.873265
H 4.440948 0.088395 3.351184
H 4.294730 1.254666 2.011577
H 2.879248 0.903970 3.049624
H 5.343984 -1.623484 1.580925
H 4.271701 -2.062169 0.209222
H 5.043534 -0.442363 0.274257
H -0.783561 0.656060 -3.723906
H 0.237750 -0.769687 -3.348954
H -0.983844 -0.211775 -2.172236
H 1.320500 1.910833 -4.215453
H 2.571206 2.168567 -2.969763
H 2.375243 0.552712 -3.718806
H -0.462398 2.824479 -2.473217
H -0.546042 2.020840 -0.874218
H 0.882818 3.010112 -1.314750
H -4.821397 -2.414911 -2.087643
H -4.864151 -0.743600 -1.455530
H -3.542756 -1.245079 -2.544684
H -4.895782 -3.372321 0.280569
H -3.722386 -2.796370 1.507006
H -5.008512 -1.706082 0.901008

H -3.053963 -4.017612 -1.360123
H -1.714639 -2.874754 -1.693524
H -1.886279 -3.598599 -0.073593
H 0.219011 2.303479 3.501988
H 0.114865 0.531682 3.279015
H 0.694329 1.558777 1.943330
H -1.516762 3.833072 2.556689
H -0.918657 3.326252 0.944852
H -2.660598 3.242579 1.315265
H -2.230680 2.088368 4.266352
H -3.487892 1.591352 3.105830
H -2.364603 0.368425 3.777157
H -5.293932 1.463728 1.417046
H -6.575273 3.228352 0.193254
H -5.767704 4.032278 -2.033780
H -3.695580 3.047501 -3.031548
H -2.439201 1.279004 -1.792661
H -3.616149 -0.072542 1.547375
Pd 1.426151 -3.307881 -1.099775

41-Pd

C	3.784844	-2.118830	0.389771
C	3.465553	-0.881390	-0.200899
C	4.444563	-0.189236	-0.940324
C	5.731356	-0.727742	-1.080440
C	6.044782	-1.966522	-0.495226
C	5.069333	-2.662550	0.237152
C	2.101416	-0.307640	-0.041750
N	1.592669	0.264026	1.049716
C	2.312612	0.884627	2.168612
C	3.001272	-0.150907	3.079626
N	1.171879	-0.203297	-1.017444
C	0.999490	-1.022617	-2.223386
C	2.171164	-0.925683	-3.219991
Si	0.000086	0.855783	-0.000216
N	-1.171619	-0.203171	1.017320
C	-0.999796	-1.021224	2.224141
C	-2.171565	-0.922459	3.220471
N	-1.592505	0.263699	-1.049866
C	-2.312326	0.883419	-2.169290
C	-3.001220	-0.152849	-3.079288
C	-2.101225	-0.307660	0.041753
C	-3.465381	-0.881394	0.201062
C	-4.444866	-0.188340	0.939002
C	-5.731656	-0.726845	1.079220
C	-6.044613	-1.966481	0.495577
C	-5.068684	-2.663395	-0.235315
C	-3.784189	-2.119709	-0.388020
C	-3.279493	1.983988	-1.691162
C	-0.689181	-2.485769	1.854735
C	0.688147	-2.486570	-1.852270
C	3.280036	1.984548	1.689528
H	0.108610	-0.597965	-2.707054
H	1.516096	1.379285	2.748626
H	3.024223	-2.646122	0.968373
H	5.308692	-3.625761	0.692607

H	7.045955	-2.387371	-0.609708
H	6.488327	-0.182861	-1.648415
H	4.187235	0.766884	-1.398022
H	0.483446	-3.080136	-2.759030
H	1.548073	-2.936809	-1.330023
H	-0.190154	-2.530302	-1.191361
H	1.871730	-1.389279	-4.174553
H	2.431620	0.127406	-3.406799
H	3.063518	-1.449368	-2.849060
H	3.683622	2.539898	2.552953
H	4.122554	1.547129	1.130965
H	2.724862	2.677992	1.034837
H	3.357822	0.344303	3.997871
H	2.296337	-0.949622	3.363199
H	3.865404	-0.610187	2.577786
H	-1.515743	1.377376	-2.749814
H	-3.682831	2.538805	-2.555047
H	-4.122194	1.547225	-1.132362
H	-2.724177	2.677747	-1.036918
H	-3.357763	0.341541	-3.997976
H	-2.296413	-0.951934	-3.362135
H	-3.865377	-0.611535	-2.576952
H	-0.108736	-0.596511	2.707427
H	-1.872585	-1.385152	4.175613
H	-2.431385	0.131012	3.406012
H	-3.064182	-1.446002	2.849977
H	-0.484855	-3.078387	2.762199
H	-1.549271	-2.936191	1.332924
H	0.189186	-2.530725	1.193978
H	-3.023223	-2.647707	-0.965525
H	-5.307669	-3.627267	-0.689564
H	-7.045789	-2.387305	0.610129
H	-6.488987	-0.181279	1.646056
H	-4.187934	0.768461	1.395504
Pd	-0.000097	3.043616	-0.000467

42-Pd

C	2.911255	-2.714669	-0.589305
C	2.082962	-2.317608	0.641505
N	1.598979	-0.920734	0.598061
Si	-0.093646	-0.399440	-0.282245
Pd	-0.603977	-2.174677	-1.502602
C	2.747939	-2.743855	1.968557
C	2.189309	0.189784	0.113984
N	1.200045	0.936913	-0.465754
C	0.998232	2.404135	-0.428563
C	1.677550	3.091777	0.766543
N	3.530448	0.526444	0.141750
C	4.313866	0.200534	1.359400
C	4.575626	1.443542	2.243282
C	4.126100	1.130145	-1.080962
C	5.101773	2.293045	-0.828151
C	4.767652	0.066243	-2.000511
N	-1.205931	-0.082744	1.179612
C	-2.219056	0.450632	0.430465
N	-3.579425	0.335384	0.760340

C	-4.447172	1.537326	0.779899
C	-5.173660	1.653097	2.142495
C	1.334318	3.124579	-1.754533
C	-1.123125	-0.318184	2.630983
C	0.211689	0.236718	3.178208
C	-2.253789	0.327169	3.451996
N	-1.675268	0.852049	-0.723827
C	-2.398212	1.221935	-1.936683
C	-1.645269	0.736231	-3.188227
C	-2.563202	2.757141	-2.003410
C	-4.215636	-1.004502	0.588284
C	-4.340120	-1.416461	-0.897841
C	-3.484743	-2.141456	1.330664
C	-5.504333	1.637885	-0.344427
C	5.621952	-0.570418	1.106952
H	1.135116	-2.880805	0.561003
H	-0.089299	2.498117	-0.295571
H	2.674105	-3.839689	2.065223
H	3.818104	-2.487100	2.013049
H	2.234762	-2.288219	2.830128
H	3.118785	-3.797823	-0.565352
H	2.321644	-2.486227	-1.493315
H	3.867629	-2.177358	-0.628994
H	0.800594	4.089088	-1.786392
H	2.409448	3.343902	-1.855334
H	1.010472	2.521602	-2.615079
H	1.349766	4.143073	0.817139
H	1.403618	2.592338	1.707614
H	2.770371	3.075733	0.671706
H	-1.139918	-1.409740	2.802874
H	0.296134	-0.007763	4.250501
H	1.068076	-0.183712	2.640422
H	0.225502	1.334157	3.071445
H	-2.058839	0.137333	4.520036
H	-2.253251	1.417572	3.290037
H	-3.245548	-0.052044	3.194255
H	-3.391418	0.752623	-1.936544
H	-2.167124	1.092329	-4.092518
H	-0.618137	1.133556	-3.193686
H	-1.576291	-0.362474	-3.198511
H	-3.117603	3.040362	-2.913790
H	-3.107751	3.146712	-1.131160
H	-1.572377	3.237687	-2.036537
H	-3.763247	2.394635	0.692653
H	-5.836351	2.533976	2.143106
H	-5.798108	0.762856	2.322879
H	-4.459517	1.750226	2.969141
H	-6.078009	2.569774	-0.214276
H	-5.057811	1.648843	-1.345756
H	-6.213108	0.797207	-0.284631
H	-5.224542	-0.899246	1.020419
H	-4.848095	-2.393322	-0.970313
H	-4.913734	-0.685176	-1.482509
H	-3.327518	-1.521784	-1.328348
H	-4.063869	-3.069273	1.195646
H	-2.485183	-2.293434	0.891859

H	-3.389033	-1.950815	2.407348
H	3.655243	-0.443274	1.948230
H	3.276862	1.529619	-1.639904
H	5.385051	2.722660	-1.802279
H	4.650078	3.089119	-0.220533
H	6.024176	1.956742	-0.332772
H	5.084193	0.547869	-2.940764
H	5.649583	-0.400974	-1.541077
H	4.035525	-0.716506	-2.240907
H	6.060475	-0.846307	2.079435
H	5.448073	-1.489968	0.532946
H	6.360049	0.043424	0.570326
H	4.999905	1.110026	3.205039
H	5.287698	2.142684	1.784344
H	3.635276	1.974718	2.444292

43-Pd

C -2.802795 -0.669998 0.037238
Si -4.594340 -1.035421 -0.265972
C -5.535929 0.506588 -0.902459
P -2.043070 0.106497 1.438015
C -2.287080 -0.940880 2.976228
C -2.922468 1.671327 1.943324
P -1.546579 -0.615033 -1.170709
C -1.983244 0.293982 -2.735435
Si -0.000320 0.636480 0.000060
P 1.546245 -0.614674 1.170851
C 1.048960 -2.282611 1.843935
C 2.802321 -0.670622 -0.037139
Si 4.593868 -1.035548 0.266637
C 5.535118 0.506755 0.902937
C 1.983188 0.295279 2.734990
C -1.049342 -2.283446 -1.842569
C -4.774672 -2.404044 -1.594183
C -5.447429 -1.608810 1.346651
P 2.042834 0.105197 -1.438502
C 2.287547 -0.943055 -2.976042
C 2.922711 1.669639 -1.944305
C 4.774247 -2.403777 1.595265
C 5.447446 -1.609154 -1.345644
H -5.837839 -2.614959 -1.805111
H -4.307750 -2.106027 -2.549918
H -4.301999 -3.347479 -1.271388
H -6.608228 0.301629 -1.074387
H -5.463035 1.336681 -0.178604
H -5.105494 0.866515 -1.853326
H -6.511175 -1.846716 1.169871
H -4.962482 -2.507768 1.763045
H -5.412418 -0.822141 2.120530
H 6.511212 -1.846749 -1.168557
H 4.962818 -2.508326 -1.761943
H 5.412408 -0.822672 -2.119711
H 6.607466 0.302011 1.074824
H 5.462037 1.336748 0.178989
H 5.104691 0.866724 1.853792
H 5.837418 -2.614431 1.806442

H 4.307110 -2.105593 2.550844
H 4.301807 -3.347388 1.272639
H -2.258608 1.323030 -2.463225
H -1.119464 0.318334 -3.419864
H -2.830100 -0.197417 -3.242115
H -1.949238 -2.809017 -2.200240
H -0.336245 -2.175549 -2.673963
H -0.586640 -2.877061 -1.040251
H -1.757481 -0.492782 3.834272
H -3.356733 -1.025601 3.227266
H -1.891699 -1.950370 2.790835
H -2.495477 2.058209 2.883916
H -2.748733 2.414989 1.149142
H -4.004635 1.504908 2.079761
H 2.496131 2.056204 -2.885214
H 2.748862 2.413683 -1.150498
H 4.004896 1.502960 -2.080316
H 1.758303 -0.495384 -3.834534
H 3.357291 -1.027972 -3.226628
H 1.892040 -1.952441 -2.790309
H 0.336305 -2.174114 2.675627
H 0.585773 -2.876644 1.042204
H 1.948940 -2.808132 2.201465
H 2.829993 -0.195973 3.241902
H 2.258733 1.324103 2.462115
H 1.119488 0.320235 3.419502
Pd 0.000651 2.823734 -0.000665

44-Pd
C 0.541878 3.136576 0.000000
C -0.945872 2.735864 0.000000
C -1.617852 3.311284 1.269092
N -1.083470 1.249915 0.000000
C -2.360625 0.681306 0.000000
C -2.360649 -0.681311 0.000000
N -1.083467 -1.249912 0.000000
C -0.945884 -2.735805 0.000000
C -1.617852 -3.311242 -1.269103
Si 0.174269 -0.000008 0.000000
C -1.617852 3.311284 -1.269092
C 0.541845 -3.136685 0.000000
C -1.617852 -3.311242 1.269103
H -3.246777 1.310548 0.000000
H -3.246767 -1.310599 0.000000
H -1.513344 4.408066 1.280802
H -2.690740 3.066968 1.300682
H -1.138112 2.898116 2.169755
H 0.612514 4.235973 0.000000
H 1.058481 2.743421 0.888990
H 1.058481 2.743421 -0.888990
H -1.513344 4.408066 -1.280802
H -1.138112 2.898116 -2.169755
H -2.690740 3.066968 -1.300682
H 0.612313 -4.236080 0.000000
H 1.058511 -2.743571 -0.888994
H 1.058511 -2.743571 0.888994

H -1.513419 -4.408030 -1.280786
H -2.690730 -3.066868 -1.300744
H -1.138078 -2.898132 -2.169778
H -1.513419 -4.408030 1.280786
H -1.138078 -2.898132 2.169778
H -2.690730 -3.066868 1.300744
Pd 2.329058 0.000003 0.000000

45-Pd
C 3.374226 -1.225878 -0.952716
C 2.649928 -0.737784 0.160358
C 3.301033 -0.066343 1.219328
C 4.696340 0.093437 1.149544
C 5.446501 -0.388826 0.063784
C 4.767118 -1.047344 -0.976557
N 1.227485 -0.921812 0.207129
Si -0.004450 0.317546 -0.072306
N -1.235130 -0.938982 0.098454
C -0.686755 -2.203356 0.355970
C 0.676593 -2.195489 0.405675
C 2.521841 0.470347 2.402892
C 6.947615 -0.181086 -0.000377
C 2.659226 -1.895807 -2.108513
C -2.657848 -0.749128 0.080745
C -3.327032 -0.620617 -1.155786
C -4.721739 -0.442217 -1.144247
C -5.452227 -0.387057 0.054926
C -4.754743 -0.516192 1.269304
C -3.361394 -0.690297 1.305720
C -2.561933 -0.670816 -2.462593
C -2.622513 -0.782292 2.624798
C -6.953083 -0.167557 0.043089
H -1.343740 -3.059996 0.487686
H 1.331267 -3.045323 0.583502
H -5.305949 -0.472855 2.213254
H -5.249035 -0.348672 -2.097963
H -3.254553 -0.708667 -3.317520
H -1.918944 0.218629 -2.576296
H -1.898807 -1.550281 -2.503064
H -2.053245 -1.722357 2.710180
H -1.888825 0.037301 2.714465
H -3.323922 -0.718083 3.470521
H -7.395358 -0.483538 -0.915112
H -7.445773 -0.728120 0.854214
H -7.199986 0.899881 0.186175
H 5.331694 -1.423195 -1.834976
H 5.208936 0.603804 1.969949
H 3.205718 0.796689 3.201710
H 1.897818 1.330694 2.105001
H 1.837850 -0.292357 2.809658
H 2.191820 -2.848249 -1.807996
H 1.843880 -1.253537 -2.482549
H 3.358253 -2.097375 -2.934320
H 7.369307 -0.003474 1.001662
H 7.454457 -1.055993 -0.439489
H 7.201784 0.692457 -0.627299

Pd 0.011179 2.439964 -0.389353

46-Pd
C -3.336024 -0.653850 1.242263
C -2.653164 -0.763507 0.010250
C -3.332045 -0.691100 -1.226722
C -4.727874 -0.516075 -1.211112
C -5.425720 -0.412040 0.000473
C -4.731791 -0.479298 1.216902
N -1.229603 -0.950670 0.015081
C -0.682472 -2.240791 0.033190
C 0.682587 -2.240767 0.033364
N 1.229636 -0.950556 0.015657
Si -0.000045 0.318453 -0.002043
C -2.567735 -0.781457 -2.531368
C -2.575985 -0.704993 2.551534
C 2.653202 -0.763361 0.010554
C 3.332114 -0.693453 -1.226551
C 4.727961 -0.518568 -1.211264
C 5.425784 -0.412137 0.000126
C 4.731818 -0.476851 1.216668
C 3.336028 -0.651250 1.242359
C 2.567774 -0.786128 -2.531005
C 2.576029 -0.699917 2.551750
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H 6.509640 -0.277343 -0.003945
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H 1.340591 -3.106704 0.045690
H -5.271840 -0.394638 2.163179
H -5.264882 -0.460064 -2.161249
H -3.259201 -0.814119 -3.387214
H -1.902471 0.090362 -2.654297
H -1.925331 -1.676554 -2.559846
H -1.907906 0.167879 2.648750
H -3.270256 -0.707798 3.405724
H -1.937138 -1.601168 2.610922
H 5.264995 -0.464473 -2.161500
H 5.271860 -0.390357 2.162784
H 3.270336 -0.700732 3.405913
H 1.907644 0.172907 2.647177
H 1.937527 -1.596223 2.613015
H 1.925946 -1.681681 -2.558262
H 1.901892 0.085070 -2.654994
H 3.259180 -0.819466 -3.386869
Pd -0.000068 2.463533 -0.031130

47-Pd
C 3.261100 1.423740 -0.401272
C 2.646860 0.173502 -0.663118
C 3.382059 -1.036005 -0.668317
C 4.761566 -0.970951 -0.395629
C 5.390005 0.253029 -0.137310
C 4.643241 1.438748 -0.140929
N 1.228287 0.132279 -0.884927
Si -0.000009 -0.140565 0.352933
N -1.228294 0.132392 -0.884827

C -0.682869 0.422536 -2.141850
C 0.682808 0.422483 -2.141850
C 2.708333 -2.384943 -0.908148
C 2.550334 -3.146608 0.429577
C 2.439105 2.709337 -0.312980
C 3.119871 3.911069 -1.003258
C -2.646905 0.173465 -0.663059
C -3.261170 1.423634 -0.401068
C -4.643315 1.438534 -0.140659
C -5.390014 0.252780 -0.137216
C -4.761526 -0.971136 -0.395744
C -3.382011 -1.036091 -0.668423
C -2.439224 2.709275 -0.312759
C -2.136317 3.029538 1.171294
C -2.708169 -2.384962 -0.908312
C -3.463951 -3.246018 -1.945052
C -2.550228 -3.146707 0.429365
C -3.119766 3.910800 -1.003617
C 3.464238 -3.246072 -1.944730
C 2.135740 3.029315 1.171061
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H 6.461728 0.283528 0.072503
H -1.341629 0.619929 -2.984314
H 1.341531 0.619830 -2.984371
H -5.344828 -1.893615 -0.382898
H -5.136085 2.388413 0.073836
H -1.477456 2.541197 -0.818767
H -1.699827 -2.197691 -1.305742
H 5.135968 2.388691 0.073385
H 5.344909 -1.893403 -0.382669
H 1.700007 -2.197796 -1.305680
H 1.477510 2.541406 -0.819364
H -2.906608 -4.178315 -2.133154
H -4.467355 -3.523522 -1.582941
H -3.581018 -2.708054 -2.899529
H -2.053969 -4.117638 0.260556
H -1.941365 -2.558037 1.138026
H -3.536851 -3.333469 0.885851
H -2.446506 4.783203 -0.980008
H -3.362265 3.682826 -2.053993
H -4.052132 4.196451 -0.489956
H -1.502939 3.929633 1.248785
H -3.074799 3.213588 1.720790
H -1.612728 2.188378 1.653906
H 2.906993 -4.178462 -2.132655
H 3.581238 -2.708262 -2.899302
H 4.467673 -3.523399 -1.582573
H 2.054319 -4.117665 0.260766
H 3.536926 -3.333110 0.886240
H 1.941212 -2.558038 1.138092
H 1.502296 3.929368 1.248533
H 1.612088 2.188061 1.653451
H 3.074082 3.213340 1.720811
H 2.446587 4.783446 -0.979549
H 4.052079 4.196559 -0.489211
H 3.362696 3.683439 -2.053634

Pd 0.000036 -0.813750 2.391377

48-Pd
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C -2.742164 -0.866897 -0.012028
C -3.391696 -1.648487 -1.181901
C -3.305630 -1.382740 1.335621
N -1.269339 -1.042035 -0.052299
Si -0.000093 0.153630 -0.000712
N 1.269443 -1.041675 0.051766
C 2.742337 -0.866617 0.011554
C 3.390940 -1.643466 1.185022
C -0.734115 -2.389471 0.227982
C 0.734527 -2.389710 -0.226000
C 3.306617 -1.388139 -1.333547
C 3.114926 0.622699 0.158274
H -1.296667 -3.168161 -0.310526
H 1.297266 -3.167257 0.314014
H -4.394976 -1.222982 1.373077
H -3.115154 -2.459846 1.465261
H -2.838627 -0.839286 2.172516
H -4.212800 0.716027 -0.174062
H -2.707824 1.221190 0.663936
H -2.712170 1.033425 -1.103289
H -4.483366 -1.497718 -1.169722
H -2.993471 -1.286841 -2.142562
H -3.202844 -2.730755 -1.106597
H 4.212746 0.717265 0.167309
H 2.707855 1.218447 -0.673221
H 2.711726 1.038302 1.094745
H 4.395913 -1.228071 -1.371007
H 3.116667 -2.465870 -1.458595
H 2.839938 -0.848519 -2.173092
H 4.482731 -1.493445 1.172761
H 2.992483 -1.277472 2.143930
H 3.201361 -2.725918 1.114190
H 0.797317 -2.617475 -1.307799
H -0.796768 -2.615215 1.310215
Pd -0.000119 2.306992 0.000255

49-Pd
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C -2.627056 1.213856 0.111465
C -3.085271 2.111054 1.289420
C -3.123948 1.816204 -1.226441
N -1.145515 1.113078 0.113288
Si -0.116441 -0.285010 0.003750
N 1.366605 0.644526 -0.030816
C 2.751380 0.113863 0.157783
C 3.592675 0.319435 -1.129188
C -0.384093 2.336661 -0.168091
C 1.107794 2.095538 0.172604
C 1.948837 3.070953 -0.674510
C 3.437758 0.789481 1.371381
C 2.730089 -1.406617 0.441481
H -0.751788 3.192437 0.420528

H -4.224813 1.860124 -1.232420
H -2.741681 2.838449 -1.374477
H -2.789673 1.189454 -2.068681
H -4.361232 -0.065477 0.329289
H -2.997657 -0.849578 -0.537108
H -2.922487 -0.647676 1.227610
H -4.185812 2.158324 1.313972
H -2.726258 1.692278 2.242330
H -2.708700 3.141325 1.192015
H 3.768102 -1.752231 0.574740
H 2.156317 -1.636246 1.352315
H 2.273853 -1.963642 -0.391349
H 4.436955 0.349079 1.513665
H 3.562449 1.873230 1.238658
H 2.845675 0.615172 2.284145
H 4.586280 -0.142365 -1.001895
H 3.086187 -0.166563 -1.977550
H 3.739471 1.378855 -1.372303
H 1.268130 2.337024 1.240982
H -0.475333 2.610109 -1.238625
H 1.538114 4.088323 -0.555811
H 3.003619 3.100520 -0.371139
H 1.892084 2.793921 -1.738447
Pd -0.558364 -2.391407 -0.120296

50-Pd
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C -2.913261 0.094654 0.409747
C -3.385938 0.411319 1.850558
C -3.400826 1.204764 -0.552265
N -1.424629 0.024408 0.375976
C -0.690175 1.089742 1.096353
C 0.776941 1.128156 0.587269
C 0.993707 2.152991 -0.596614
C 0.119451 1.823246 -1.823872
Si -0.316256 -1.122134 -0.276827
P -0.551776 -2.775202 -1.595896
N 1.115839 -0.278864 0.239675
C 2.382132 -0.984795 0.658095
C 3.104540 -1.558157 -0.583439
C 3.346236 -0.069829 1.439648
C 2.006094 -2.160249 1.599559
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H -3.121798 0.958173 -1.587747
H -4.635652 -1.154084 0.034431
H -3.245648 -1.527862 -1.035545
H -3.220118 -2.055295 0.660254
H -4.486068 0.394412 1.879049
H -3.004806 -0.346250 2.553285
H -3.053450 1.405138 2.187318
H 2.914787 -2.665200 1.966091
H 1.435608 -1.784682 2.464481

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H 4.239024 -0.660829 1.693798
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H 3.954474 -2.182225 -0.260728
H 2.409862 -2.176294 -1.171765
H 3.494173 -0.756511 -1.227542
H 1.409317 1.474861 1.416180
H -1.187888 2.055282 0.938142
H 2.598971 2.825598 -1.901846
H 3.128154 2.516655 -0.231142
H 2.790553 1.147048 -1.334200
H 0.993900 4.320778 -0.840241
H -0.419998 3.736172 0.055141
H 1.177819 3.797432 0.854306
H 0.294117 2.571890 -2.614064
H 0.383293 0.836767 -2.240323
H -0.949974 1.825717 -1.574303
H -0.411020 -3.684706 -0.485092

51-Pd
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C -2.829593 2.344834 1.119775
C -2.892204 2.186595 -1.408981
N -1.052994 1.138741 -0.111168
Si -0.212172 -0.378132 -0.040150
N 1.379270 0.359842 -0.074479
C 2.683257 -0.370208 -0.136157
C 3.385169 -0.131889 -1.501274
C -0.118638 2.228738 -0.413085
C 1.279047 1.846762 0.145029
C 1.304092 2.181811 1.660724
C 2.305340 2.720997 -0.604334
C 3.639243 0.018590 1.018593
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H -0.441425 3.176211 0.047111
H -3.974012 2.394423 -1.411881
H -2.360294 3.146231 -1.505421
H -2.648665 1.559994 -2.281648
H -4.405356 0.424395 0.027533
H -3.146250 -0.501956 -0.857744
H -3.082103 -0.402275 0.913876
H -3.907356 2.575140 1.140396
H -2.560234 1.819813 2.049418
H -2.282140 3.299852 1.085280
H 3.435761 -2.398308 -0.049987
H 1.950154 -2.155550 0.925741
H 1.836393 -2.280552 -0.843675
H 4.564560 -0.573163 0.929936
H 3.918866 1.079709 0.998384
H 3.174851 -0.204446 1.991463
H 4.253153 -0.806338 -1.591251
H 2.682322 -0.353481 -2.319366
H 3.748905 0.896394 -1.615908
H -0.054603 2.393130 -1.506912

H 2.027884 3.777788 -0.454527
H 3.330978 2.593532 -0.234603
H 2.284713 2.509906 -1.683004
H 1.187359 3.269463 1.805742
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H 2.241801 1.868204 2.134114
Pd -0.951997 -2.400256 0.074784

52-Pd
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C 0.714681 1.817312 -0.608114
C -0.715990 1.816867 -0.608264
C -1.417683 3.033040 -0.662443
C -0.704529 4.240355 -0.714365
C 0.701704 4.240783 -0.714163
N 1.247286 0.521173 -0.588807
C 2.690156 0.253683 -0.579727
C 3.345016 0.127442 0.826997
C 2.690261 -1.017838 1.626133
N -1.247804 0.520403 -0.589017
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C -3.345310 0.125360 0.826941
C -3.230170 1.439489 1.625933
Si 0.000121 -0.718090 -0.639572
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C 3.229178 1.441547 1.625937
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H 1.248123 5.185211 -0.751058
H 2.504522 3.037828 -0.656992
H 2.847993 -0.699319 -1.111044
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H 5.365138 -0.294023 1.551276
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H 2.689448 -1.957252 1.048034
H -2.847690 -0.701197 -1.111065
H -3.205412 1.038160 -1.156389
H -3.680832 1.311965 2.624367
H -2.178191 1.734680 1.754160
H -3.758698 2.261619 1.116175
H -5.365196 -0.297434 1.551150
H -5.326453 0.590020 0.001830
H -4.945483 -1.157065 0.042531
H -3.238411 -1.183071 2.568895
H -2.689194 -1.959105 1.048122
H -1.644173 -0.783017 1.874884
Pd 0.001264 -2.862568 -0.562133

53-Pd
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C 3.083396 0.538154 -0.539910
C 1.686286 0.401691 -0.523001
C 0.853994 1.564082 -0.531196
C 1.443791 2.837971 -0.555386
C 2.841522 2.952817 -0.569583
N 0.942015 -0.785247 -0.542842
Si -0.789996 -0.490444 -0.643621
N -0.510844 1.243601 -0.558913
C -1.564737 2.264233 -0.568360
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C -2.666698 1.501956 1.596699
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C 1.563938 -2.113662 -0.526116
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H 3.717861 -0.347890 -0.531627
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H 2.518800 -2.070293 -1.076061
H 2.602619 -4.621101 1.627725
H 1.690601 -4.774238 0.099788
H 3.339549 -4.081097 0.093757
H 2.924356 -2.326083 2.710440
H 3.780956 -1.836461 1.224048
H 2.426321 -0.849648 1.834524
H 0.625173 -3.398336 2.594186
H 0.061403 -1.855184 1.897455
H -0.287972 -3.378084 1.050382
H -2.417793 1.848635 -1.129458
H -1.203843 3.146191 -1.123455
H -1.359358 3.640881 2.661028
H -0.125315 2.665522 1.811855
H -0.584708 4.270065 1.182254
H -3.613991 4.103583 1.534052
H -2.821710 4.609114 0.015569
H -4.033105 3.293413 -0.001634
H -3.143392 1.843968 2.530417
H -3.417216 0.968656 0.989323
H -1.878689 0.779164 1.859335
H 5.673570 1.136430 -1.082457
H 5.501451 2.910550 -0.985786
H 5.574295 1.937327 0.501139
Pd -2.528566 -1.749202 -0.638976

54-Pd
C 1.069974 4.040168 -0.711762
N 1.654256 2.823612 -0.672457
C 0.835495 1.768645 -0.628462

C -0.596355 1.853105 -0.623269
C -1.176427 3.126183 -0.669613
C -0.318579 4.240087 -0.712953
N 1.292124 0.447926 -0.613274
Si -0.028870 -0.715033 -0.659637
N -1.206180 0.600328 -0.606634
C -2.662794 0.424340 -0.582899
C -3.307017 0.345677 0.831582
C -2.683625 -0.804753 1.648311
C 2.732150 0.143280 -0.588498
C 3.332594 -0.066845 0.832088
C 3.014322 1.130431 1.750932
C 2.796400 -1.366847 1.465099
C 4.862497 -0.185875 0.648768
C -3.137182 1.671642 1.600885
C -4.811005 0.065356 0.614546
H -2.258978 3.249008 -0.663771
H -0.727418 5.251374 -0.744690
H 1.752483 4.894189 -0.743474
H 2.890410 -0.775597 -1.175875
H 3.254626 0.974032 -1.084455
H 5.350072 -0.370399 1.619883
H 5.115199 -1.021442 -0.026298
H 5.278529 0.742699 0.223515
H 3.508159 0.994129 2.727606
H 3.357082 2.073309 1.300296
H 1.929517 1.213538 1.922576
H 3.246179 -1.517690 2.460815
H 1.701221 -1.336115 1.584584
H 3.038288 -2.240287 0.836139
H -2.884315 -0.518026 -1.110253
H -3.132141 1.241918 -1.155882
H -3.590525 1.586178 2.602354
H -2.073848 1.926379 1.722653
H -3.634289 2.502373 1.072836
H -5.334457 0.020776 1.583185
H -5.276919 0.861731 0.009108
H -4.961350 -0.896720 0.096303
H -3.236397 -0.938635 2.592967
H -2.706962 -1.752522 1.084185
H -1.631592 -0.592210 1.894286
Pd -0.227228 -2.847221 -0.552079

55-Pd
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C -2.715850 0.899205 -0.021709
C -4.086162 0.594284 -0.022791
C -4.545723 -0.634438 -0.588647
C -3.618212 -1.510054 -1.184551
C -0.340152 0.356588 -0.624952
C 0.631710 -0.661096 -0.514136
C 1.996797 -0.345046 -0.520297
C 2.417979 1.015975 -0.637836
C 1.453255 2.030842 -0.752342
C 0.093716 1.698705 -0.746087

N 3.811923 1.144243 -0.658837
Si 4.628762 -0.414299 -0.603120
N 3.078634 -1.232450 -0.446583
C 2.904456 -2.683046 -0.309892
C 2.849429 -3.220253 1.150698
C 4.143744 -2.855068 1.905659
N -5.134168 1.355634 0.502271
C -4.888089 2.655051 1.143955
C -4.931524 3.902312 0.210197
C -6.330459 4.048582 -0.421432
N -5.928757 -0.785889 -0.470768
C -6.612069 -1.985724 -0.974824
C -6.765566 -3.161473 0.037981
C -7.628654 -2.725922 1.239031
C 4.486751 2.443785 -0.746284
C 4.808223 3.127438 0.615543
C 3.523662 3.438467 1.410311
C 5.731438 2.230273 1.464782
C 5.542443 4.446007 0.283671
C 1.632670 -2.663286 1.917703
C 2.733015 -4.757735 1.049246
Si -6.746282 0.593010 0.331128
C -4.644810 5.130530 1.103567
C -3.871418 3.823608 -0.907348
C -7.483225 -4.302684 -0.717297
C -5.397720 -3.660176 0.546515
H 0.312178 -1.693014 -0.383939
H -0.648876 2.489481 -0.865822
H 1.761139 3.070862 -0.851511
H 5.439754 2.282178 -1.276263
H 3.877731 3.123749 -1.364927
H 5.796911 4.985298 1.210432
H 6.477749 4.248461 -0.267124
H 4.909078 5.104728 -0.334704
H 3.784193 3.899028 2.377910
H 2.876941 4.141938 0.860984
H 2.946777 2.522072 1.603660
H 6.044473 2.767980 2.375206
H 5.216786 1.306490 1.771935
H 6.631454 1.937548 0.898561
H 3.760410 -3.163247 -0.811854
H 1.992438 -2.987268 -0.850205
H 1.638088 -3.042448 2.953299
H 1.651727 -1.563960 1.949182
H 0.687308 -2.976670 1.445505
H 2.676742 -5.204117 2.055286
H 1.824455 -5.048192 0.494488
H 3.607524 -5.186040 0.530696
H 4.152037 -3.340674 2.895606
H 5.036329 -3.177870 1.343694
H 4.221358 -1.767236 2.056753
H -2.360439 1.817036 0.441911
H -3.953707 -2.442602 -1.635783
H -1.551779 -1.847204 -1.688767
H -5.659938 2.793634 1.919105
H -3.915972 2.620371 1.662850

H -4.666248 6.054118 0.502621
H -5.399559 5.223634 1.902845
H -3.650166 5.050183 1.574408
H -6.382633 4.976434 -1.014688
H -6.554578 3.202628 -1.090374
H -7.112946 4.088883 0.354926
H -3.957979 4.703110 -1.567027
H -2.852493 3.812578 -0.487375
H -4.002349 2.916462 -1.515128
H -7.623992 -1.684433 -1.292428
H -6.087870 -2.346185 -1.875354
H -7.633731 -5.167112 -0.050379
H -8.471190 -3.974531 -1.082378
H -6.887181 -4.636736 -1.583576
H -7.794853 -3.581452 1.914246
H -7.133292 -1.927763 1.814275
H -8.610993 -2.350492 0.906617
H -5.544496 -4.463802 1.287274
H -4.789819 -4.065178 -0.278411
H -4.831191 -2.846099 1.022001
Pd 6.681233 -1.035319 -0.524551

56-Pd
C 2.793930 -1.654122 -2.379684
C 3.671216 -1.119276 -1.418494
C 5.065159 -1.185262 -1.623875
C 5.575041 -1.773489 -2.790605
C 4.696166 -2.308858 -3.748433
C 3.308533 -2.252097 -3.540515
P 2.940270 -0.309138 0.067679
C 3.269135 1.476797 -0.070397
C 3.970012 2.011931 -1.159196
C 4.072691 3.407384 -1.344480
C 3.480607 4.288710 -0.426024
C 2.779847 3.793538 0.695400
C 2.603715 2.374323 0.855523
C 1.231290 -0.587420 0.204184
Si -0.039946 0.726671 -0.058498
C -1.398570 -0.500277 0.193457
P -3.085377 -0.166995 0.044916
C -3.869403 -1.009454 -1.392805
C -5.268156 -1.038253 -1.575629
C -5.815049 -1.661728 -2.706819
C -4.968682 -2.268384 -3.651216
C -3.576875 -2.248582 -3.465471
C -3.024529 -1.617067 -2.340496
C -0.849398 -1.848150 0.354785
C -1.569769 -3.061031 0.462931
C -0.912132 -4.291919 0.575800
C 0.494821 -4.339330 0.571165
C 1.235561 -3.157218 0.455926
C 0.601989 -1.895659 0.353723
C -4.131638 -0.686489 1.486442
C -4.174489 0.132024 2.634184
C -4.882902 -0.277444 3.772507
C -5.553695 -1.511420 3.781093

C -5.516912 -2.331552 2.642925
C -4.811994 -1.921842 1.501065
C -3.345063 1.633994 -0.172008
C -4.132064 2.137855 -1.227401
C -4.286121 3.522225 -1.395365
C -3.657117 4.416347 -0.512734
C -2.866618 3.921903 0.535128
C -2.704169 2.538591 0.705795
C 3.977094 -0.976408 1.457398
C 4.554298 -2.261775 1.387330
C 5.285754 -2.775779 2.468453
C 5.456095 -2.009646 3.631775
C 4.896691 -0.723677 3.705636
C 4.162892 -0.210096 2.626572
H 2.323413 -3.214512 0.440001
H 1.013201 -5.298291 0.652183
H -1.494511 -5.212909 0.661299
H -2.659968 -3.042859 0.451708
H -5.923235 -0.579456 -0.832553
H -6.897822 -1.678109 -2.849137
H -5.395792 -2.758989 -4.528667
H -2.920050 -2.727668 -4.194454
H -1.946023 -1.599215 -2.176120
H -3.662433 1.094226 2.639317
H -4.911251 0.369099 4.652208
H -6.102587 -1.830835 4.669543
H -6.036034 -3.292444 2.640391
H -4.800542 -2.561665 0.618345
H -4.611676 1.455050 -1.928487
H -4.893525 3.900111 -2.220388
H -3.778083 5.493597 -0.646450
H -2.358317 4.607447 1.215832
H -2.063886 2.168105 1.504014
H 4.425759 1.346398 -1.892937
H 4.622037 3.796423 -2.203530
H 3.585367 5.368316 -0.559069
H 2.466287 4.469061 1.494041
H 2.283159 1.986863 1.825079
H 4.448579 -2.856507 0.479642
H 5.724294 -3.773592 2.397746
H 6.025890 -2.409170 4.473538
H 5.034401 -0.115637 4.602461
H 3.749438 0.795131 2.694212
H 5.744782 -0.781287 -0.871122
H 6.654605 -1.817847 -2.950886
H 5.094613 -2.771954 -4.653975
H 2.625941 -2.674565 -4.280946
H 1.718772 -1.603951 -2.199171
Pd 0.661911 2.865408 -0.015194

57-Pd
C 2.868854 -2.443426 -0.457264
C 3.406574 -1.198879 -0.849548
C 4.187342 -1.118275 -2.020307
C 4.440344 -2.276229 -2.768195
C 3.916537 -3.515357 -2.357667

C 3.127616 -3.613771 -1.201352
P 3.014203 0.283748 0.142665
C 1.318749 0.369421 0.478522
C 0.725288 1.470860 1.238637
C -0.725038 1.470830 1.238857
C -1.401853 2.520846 1.904663
C -0.703232 3.543101 2.558247
C 0.703783 3.543181 2.557954
C 1.402254 2.520983 1.904124
C -1.318686 0.369383 0.478881
P -3.014107 0.284206 0.142664
C -3.617567 1.750569 -0.793420
C -2.651421 2.613812 -1.335266
C -3.029141 3.750629 -2.075678
C -4.399787 3.997529 -2.273850
C -5.374625 3.136211 -1.740838
C -4.989672 2.015004 -0.993449
C -1.965443 4.677443 -2.630141
C 2.502336 -4.922236 -0.764203
C 4.111082 0.211835 1.638737
C 4.766417 1.350561 2.147744
C 5.525993 1.254599 3.323757
C 5.636811 0.029961 3.995945
C 4.987711 -1.120602 3.505255
C 4.232483 -1.012843 2.325050
C 5.083860 -2.443013 4.241297
C 3.618268 1.749745 -0.793608
C 4.990484 2.013689 -0.993531
C 5.375889 3.134660 -1.741035
C 4.401393 3.996238 -2.274264
C 3.030645 3.749842 -2.076177
C 2.652466 2.613244 -1.335658
C 1.967324 4.677019 -2.630752
Si -0.000054 -0.653559 -0.310272
C -3.406695 -1.198102 -0.849944
C -4.187407 -1.117062 -2.020710
C -4.440651 -2.274794 -2.768864
C -3.917134 -3.514130 -2.358608
C -3.128254 -3.612981 -1.202296
C -2.869251 -2.442860 -0.457937
C -2.503419 -4.921736 -0.765352
C -4.111352 0.212184 1.638465
C -4.233355 -1.012668 2.324379
C -4.988830 -1.120509 3.504406
C -5.637546 0.030166 3.995373
C -5.526137 1.254964 3.323592
C -4.766328 1.350999 2.147727
C -5.085780 -2.443119 4.239984
H -2.491247 2.540579 1.912028
H -1.255513 4.338549 3.065368
H 1.256187 4.338707 3.064821
H 2.491650 2.540888 1.910999
H 5.744015 1.352857 -0.561596
H 6.435623 3.342815 -1.904610
H 4.708977 4.874476 -2.848033
H 1.596290 2.397945 -1.161598

H 3.741165 -1.905747 1.936215
H 6.233418 -0.039417 4.909480
H 6.034748 2.139535 3.712522
H 4.691553 2.305606 1.627364
H 4.579885 -0.159306 -2.357362
H 5.042246 -2.211935 -3.677083
H 4.111569 -4.413582 -2.949797
H 2.235626 -2.509766 0.425985
H -4.579716 -0.157934 -2.357586
H -5.042491 -2.210151 -3.677770
H -4.112318 -4.412170 -2.950969
H -2.236057 -2.509522 0.425314
H -4.690993 2.306182 1.627669
H -6.034597 2.139980 3.712562
H -6.234320 -0.039256 4.908796
H -3.742315 -1.905639 1.935348
H -5.743470 1.354376 -0.561668
H -6.434274 3.344758 -1.904470
H -4.707017 4.875962 -2.847510
H -1.595333 2.398161 -1.161126
H 1.315461 5.050856 -1.823432
H 2.414837 5.542444 -3.143831
H 1.318450 4.148774 -3.350105
H 2.918917 -5.271902 0.196933
H 1.415112 -4.780308 -0.616534
H 2.659180 -5.714127 -1.513265
H 6.085516 -2.586031 4.678251
H 4.354214 -2.487349 5.069375
H 4.874009 -3.289383 3.568610
H -4.873501 -3.289198 3.567705
H -4.358303 -2.486981 5.069990
H -6.088463 -2.587044 4.674304
H -2.921827 -5.272648 0.194547
H -2.658593 -5.712834 -1.515601
H -1.416529 -4.779679 -0.615462
H -1.312399 5.049595 -1.823009
H -1.317827 4.149457 -3.350831
H -2.412603 5.543943 -3.141712
Pd -0.000240 -2.457729 -1.552293

58-Pd
C 1.701696 3.021910 -1.216087
Si 2.600098 1.451526 -0.605310
C 3.077084 0.458780 -2.159279
C 1.450809 0.469508 0.605910
Si 2.478997 -0.915712 1.489429
C 3.447757 -0.142132 2.943576
Si 0.003477 -0.298128 -0.371258
C -1.420195 0.395517 0.696541
Si -2.714482 -1.022730 0.940879
C -3.654057 -1.333604 -0.687690
C 0.729625 1.391233 1.665384
C -0.675067 0.821101 2.015494
Si -2.304688 1.899933 -0.157637
C -1.547844 3.572976 0.369944
C 1.381740 -2.275351 2.247138

C 3.672047 -1.791990 0.292944
C 4.197184 2.032647 0.268034
C -2.243551 1.729615 -2.054392
C -4.132753 2.091247 0.377061
C -1.912420 -2.696721 1.376128
C -3.872287 -0.608015 2.404587
H 0.594669 2.400458 1.249586
H 1.327644 1.509006 2.584493
H -1.249268 1.564504 2.596125
H -0.544653 -0.056617 2.673264
H 3.497699 1.149383 -2.912185
H 3.827432 -0.319883 -1.959304
H 2.191438 -0.035130 -2.596405
H 4.766963 2.698271 -0.404388
H 3.982378 2.596249 1.191857
H 4.853566 1.188083 0.533577
H 2.307987 3.502652 -2.003698
H 0.712909 2.799641 -1.650381
H 1.560235 3.762932 -0.412619
H 4.134396 -0.895132 3.369524
H 4.045071 0.733512 2.648944
H 2.766493 0.170466 3.752910
H 4.083129 -2.692154 0.782819
H 3.140557 -2.112537 -0.618262
H 4.520228 -1.158488 -0.011023
H 2.014518 -2.995701 2.796078
H 0.643592 -1.873752 2.960353
H 0.834431 -2.834879 1.473510
H -4.554456 2.961433 -0.157570
H -4.771147 1.223086 0.160933
H -4.206427 2.303023 1.456957
H -2.830691 2.532119 -2.535456
H -1.212378 1.786342 -2.443192
H -2.651470 0.759789 -2.380309
H -2.226980 4.377341 0.035810
H -1.465604 3.651122 1.467340
H -0.558268 3.774276 -0.060255
H -2.713337 -3.453543 1.458996
H -1.222042 -3.024372 0.580580
H -1.364010 -2.690462 2.329945
H -4.439649 -1.509767 2.695567
H -3.282217 -0.296331 3.284455
H -4.596428 0.190831 2.187904
H -4.347544 -2.184631 -0.568124
H -4.232763 -0.474429 -1.058261
H -2.912868 -1.603486 -1.463042
Pd -0.054552 -1.648957 -2.044658

59-Pd
C -5.507188 1.440728 -0.422887
C -4.310796 0.726657 -0.200362
C -4.363341 -0.555443 0.420463
C -5.613238 -1.088361 0.800498
C -6.796218 -0.365051 0.577921
C -6.743354 0.899948 -0.033717
Si -2.665975 -1.385653 0.619520

C -2.500130 -2.229579 2.316847
Si -2.563080 1.284965 -0.688627
C -2.261596 0.958640 -2.540308
C -1.492409 0.132272 0.440352
Si 0.198163 -0.219892 -0.335576
C 1.188850 0.867725 0.862165
Si 2.502744 1.875033 -0.104470
C 2.983913 3.418068 0.910839
C 0.126428 1.673943 1.674095
C -1.158705 0.818815 1.816786
Si 2.293761 -0.335498 1.885463
C 1.544230 -2.063257 2.190520
C 3.828999 -0.423853 0.780460
C 3.927314 0.627988 -0.178470
C 5.020040 0.650558 -1.069585
C 6.004289 -0.350403 -1.018795
C 5.908083 -1.385327 -0.072190
C 4.826134 -1.420019 0.822636
C 2.678286 0.458873 3.576446
C 1.924430 2.428946 -1.831511
C -2.394654 -2.663033 -0.762502
C -2.297205 3.138352 -0.341831
H -0.124352 2.608817 1.145908
H 0.503040 1.965973 2.669497
H -0.973788 0.041003 2.578289
H 1.764643 0.564206 4.186983
H 3.392086 -0.159475 4.147813
H 3.120638 1.461135 3.454695
H 0.636792 -2.001998 2.815604
H 1.275909 -2.552697 1.238165
H 2.262144 -2.718071 2.715790
H 2.106763 4.064454 1.089642
H 3.400257 3.138221 1.892703
H 3.742600 4.022297 0.383778
H 1.030987 3.075954 -1.769221
H 2.708099 3.003329 -2.356353
H 1.668072 1.546671 -2.442607
H -1.996575 1.432815 2.193141
H 5.103090 1.444835 -1.817853
H 6.843428 -0.328689 -1.718819
H 6.672414 -2.165853 -0.038306
H 4.755416 -2.237608 1.546766
H -1.255885 1.289380 -2.850044
H -2.335136 -0.115290 -2.774403
H -3.006498 1.495952 -3.153837
H -1.317515 3.480499 -0.716416
H -3.073008 3.733962 -0.854523
H -2.352808 3.370618 0.733680
H -1.389650 -3.112744 -0.695954
H -3.150298 -3.467217 -0.712994
H -2.463781 -2.188148 -1.754390
H -1.502343 -2.681234 2.446683
H -2.667930 -1.521976 3.145027
H -3.244527 -3.039306 2.412984
H -5.479959 2.428108 -0.894747
H -7.664856 1.463108 -0.201919

H -7.759038 -0.782527 0.883418
H -5.669483 -2.070362 1.280784
Pd 0.925858 -1.429057 -1.951838

60-Pd
N 2.171722 -1.629063 1.730668
C 2.153285 -0.708339 0.718947
N 3.356542 -0.059816 0.812917
C 4.120007 -0.574257 1.859368
C 3.374917 -1.572795 2.437242
Si 0.820985 -0.360792 -0.666551
C 0.123161 1.319919 -0.139251
C 0.873601 2.582999 -0.229215
C 1.441439 2.971293 -1.468722
C 2.258820 4.105060 -1.563017
C 2.539697 4.876229 -0.421296
C 1.986068 4.503911 0.814959
C 1.161613 3.371966 0.908984
C 3.804083 1.013130 -0.081539
C 5.480341 -0.055647 2.208741
C 3.693806 -2.468973 3.593803
C 1.073744 -2.553873 2.035470
C -0.804256 -1.231924 -0.228823
C -1.049709 -2.681042 -0.293763
C -1.893297 -3.344572 0.635756
C -2.024330 -4.738118 0.628235
C -1.316914 -5.517027 -0.305484
C -0.474583 -4.878905 -1.230949
C -0.341994 -3.482829 -1.226109
C -1.728741 -0.246713 0.083840
C -3.185120 -0.507323 0.249524
C -3.887901 -0.047126 1.384479
C -5.255536 -0.314468 1.537645
C -5.947974 -1.039594 0.553952
C -5.260993 -1.495862 -0.583989
C -3.892930 -1.233539 -0.733278
C -1.211245 1.150423 0.161697
C -2.151115 2.291578 0.368521
C -2.089403 3.106034 1.516420
C -2.978532 4.179121 1.686132
C -3.946940 4.452307 0.708136
C -4.023598 3.641967 -0.437524
C -3.136644 2.570355 -0.602810
H -3.355421 0.529961 2.141715
H -5.781975 0.049150 2.423373
H -7.015014 -1.243268 0.670487
H -5.792479 -2.055756 -1.357177
H -3.353427 -1.592285 -1.611063
H -1.355466 2.878850 2.290526
H -2.916033 4.797948 2.584592
H -4.640246 5.286447 0.838906
H -4.777718 3.843757 -1.201866
H -3.203552 1.932708 -1.485995
H 1.247111 2.346040 -2.343592
H 2.684393 4.385079 -2.530006
H 3.182227 5.756788 -0.494368

H 2.200366 5.092344 1.710839
H 0.765427 3.067316 1.877913
H -2.434056 -2.753864 1.375703
H -2.678191 -5.220454 1.359456
H -1.421924 -6.604439 -0.309991
H 0.080426 -5.469604 -1.964421
H 0.312645 -2.983185 -1.946993
H 5.860733 -0.574760 3.099534
H 6.202691 -0.215016 1.389720
H 5.457016 1.025893 2.424505
H 3.676115 -3.532949 3.302884
H 4.698560 -2.239110 3.974924
H 2.979343 -2.338762 4.425019
H 1.253682 -3.000782 3.020216
H 0.130688 -1.997821 2.042830
H 1.009419 -3.341070 1.272412
H 4.901425 1.014427 -0.103637
H 3.406726 0.804908 -1.090965
H 3.426792 1.984962 0.261838
Pd 1.742633 -0.596096 -2.647765

61-Pd
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C -2.924176 1.679853 0.033435
C -2.971154 2.586694 1.114680
C -4.105208 3.379290 1.338195
C -5.214206 3.281628 0.480961
C -5.179534 2.383054 -0.598300
C -1.712434 0.847343 -0.201315
C -1.824020 -0.632351 -0.328619
C -3.129034 -1.326580 -0.168958
C -3.952727 -1.089745 0.954470
C -5.155933 -1.789080 1.122203
C -5.562852 -2.734124 0.165613
C -4.755003 -2.974198 -0.958953
C -3.549612 -2.278720 -1.122948
C -0.633681 -1.308845 -0.559135
C -0.395641 -2.757198 -0.497905
C -1.030756 -3.581736 0.467768
C -0.713090 -4.940994 0.578347
C 0.244444 -5.520927 -0.272653
C 0.883872 -4.719764 -1.233702
C 0.571318 -3.358209 -1.344961
Si 0.719379 -0.020928 -0.860228
C -0.433787 1.374192 -0.307699
C -0.052647 2.797747 -0.250379
C -0.802344 3.823819 -0.876059
C -0.382911 5.159040 -0.822231
C 0.795786 5.512083 -0.141579
C 1.557416 4.508626 0.478674
C 1.140817 3.171288 0.417661
C 1.978006 -0.228553 0.642345
N 1.668922 -0.421217 1.963621
C 2.825941 -0.443511 2.739385
C 3.883390 -0.259059 1.877463
N 3.344566 -0.136719 0.597034

C 0.269686 -0.473991 2.476310
C 0.001532 -1.723782 3.329239
C 4.117378 0.142652 -0.645155
C 4.539208 1.616801 -0.697964
C 5.346479 -0.217782 2.203534
C 2.870401 -0.667890 4.221422
C 5.259932 -0.857035 -0.871518
C -0.107919 0.845922 3.166896
H -3.645628 -0.345865 1.691449
H -5.778518 -1.592651 1.998463
H -6.502638 -3.276316 0.293596
H -5.064616 -3.705237 -1.709639
H -2.913682 -2.469335 -1.988837
H -2.104055 2.670631 1.771137
H -4.123241 4.074842 2.180781
H -6.098721 3.899148 0.653764
H -6.037728 2.298888 -1.269122
H -4.025216 0.878927 -1.647281
H -1.711615 3.558543 -1.414691
H -0.976753 5.929379 -1.320359
H 1.118683 6.554839 -0.101519
H 2.478838 4.766025 1.007724
H 1.739615 2.396631 0.900790
H -1.772258 -3.141064 1.133868
H -1.215913 -5.551214 1.333238
H 0.485933 -6.583171 -0.188646
H 1.626823 -5.158967 -1.904779
H 1.059426 -2.730134 -2.097080
H 5.480599 -0.065571 3.283687
H 5.855006 -1.156482 1.929443
H 5.857956 0.601344 1.679213
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H 3.863044 -0.394881 4.606302
H 2.123594 -0.062307 4.753164
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H 3.379354 -0.012242 -1.461458
H -1.188705 0.830990 3.376132
H 0.422856 0.990496 4.120783
H 0.100329 1.695582 2.502025
H -1.088057 -1.808556 3.461974
H 0.348170 -2.628696 2.809424
H 0.459572 -1.668056 4.326777
H 5.035696 1.805030 -1.662909
H 3.652363 2.264934 -0.636495
H 5.240669 1.886422 0.108336
H 5.568286 -0.777635 -1.925751
H 6.143734 -0.658852 -0.247722
H 4.915855 -1.887726 -0.693918
Pd 1.606123 0.004121 -2.872682

62-Pd
C -5.589766 1.988392 -0.688681
C -4.812391 0.891692 -1.073295
C -3.462378 0.894523 -0.683474
C -2.895278 1.992975 -0.014236
C -3.684564 3.074811 0.411387

C -5.039447 3.052072 0.067120
N -1.535338 1.710822 0.120108
C -1.245616 0.456352 -0.366307
N -2.436796 -0.034958 -0.853162
Si 0.558538 -0.670822 -0.193645
N 1.019105 -0.123377 1.459380
C 0.297001 -0.456703 2.683621
C 0.862545 -1.639844 3.528912
C 0.835630 -2.948073 2.714033
C -2.690780 -1.393949 -1.370132
C -3.359850 -2.386422 -0.361686
C -4.887732 -2.192457 -0.236269
C -0.577129 2.710174 0.630047
C -0.168581 3.837323 -0.368967
C -1.310511 4.823104 -0.692622
C 2.048421 0.826462 1.444187
C 2.554019 1.075829 0.124184
C 3.551085 2.044461 -0.064793
C 4.068993 2.755119 1.037914
C 3.568292 2.520234 2.323584
C 2.553076 1.562891 2.528087
N 1.911829 0.306988 -0.853453
C 2.346906 0.303135 -2.251443
C 3.558462 -0.602996 -2.642661
C 4.870700 -0.172790 -1.955007
C 3.281141 -2.078201 -2.300123
C 3.725792 -0.459150 -4.173156
C 2.307538 -1.364951 3.990762
C -0.054989 -1.787771 4.762899
C -3.100174 -3.799121 -0.935413
C -2.722222 -2.267107 1.035138
C 0.960930 4.618864 0.343127
C 0.358221 3.233021 -1.682709
H 2.170800 1.384212 3.531605
H 3.962281 3.072426 3.179505
H 4.855052 3.495792 0.876705
H 3.930422 2.240583 -1.065876
H 1.487431 -0.030306 -2.855631
H 2.578463 1.336906 -2.568041
H 4.579200 -1.063273 -4.522308
H 2.820793 -0.804079 -4.701974
H 3.912169 0.592127 -4.454338
H 5.685836 -0.849537 -2.263648
H 5.156474 0.852789 -2.241273
H 4.779580 -0.212416 -0.860492
H 4.124739 -2.708156 -2.632784
H 3.142990 -2.210630 -1.215921
H 2.357919 -2.430106 -2.791113
H -0.738600 -0.716359 2.405800
H 0.236478 0.440691 3.327257
H 2.696785 -2.239465 4.539074
H 2.964041 -1.170762 3.129994
H 2.354137 -0.493890 4.664338
H 0.287594 -2.619830 5.399877
H -0.052540 -0.866577 5.371478
H -1.094636 -1.996962 4.456456

H 1.245067 -3.776820 3.316925
H -0.193430 -3.208217 2.420468
H 1.427191 -2.851911 1.789683
H -5.238444 0.063750 -1.634594
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H -5.681895 3.878163 0.376100
H -3.256603 3.903643 0.969778
H -3.322066 -1.285212 -2.266505
H -1.706708 -1.796813 -1.662322
H -1.033064 3.159512 1.526775
H 0.319040 2.172656 0.941948
H -3.153308 -3.026572 1.708102
H -1.634227 -2.423753 0.965086
H -2.915199 -1.273645 1.472683
H -3.566880 -4.560234 -0.289689
H -3.523316 -3.899856 -1.949910
H -2.014475 -3.993778 -0.985840
H -5.310804 -3.024509 0.350505
H -5.143322 -1.255934 0.279498
H -5.375721 -2.197174 -1.226606
H -0.909592 5.635505 -1.320626
H -2.132660 4.344357 -1.243906
H -1.717252 5.281183 0.224547
H 0.644593 4.042722 -2.373588
H 1.235743 2.608549 -1.490730
H -0.411236 2.617281 -2.176574
H 1.310533 5.436471 -0.308198
H 0.591776 5.066945 1.281976
H 1.813649 3.966539 0.575422
Pd 0.362706 -2.759146 -0.825993

63-Pd
C -0.288926 1.873847 3.057921
C -1.510395 2.151859 2.132073
C -1.227077 1.140791 1.015821
C 0.154515 1.079863 0.882304
C 0.754254 2.024783 1.915378
C 0.424025 3.478148 1.409157
C -1.130728 3.583574 1.602407
N 0.817554 0.380635 -0.073371
Si -0.182025 -0.719425 -1.198807
P -2.124859 0.173978 -0.156948
C -3.230072 1.313630 -1.215767
C -2.262773 2.217560 -2.018955
C 2.250472 0.277142 -0.031067
C 3.020689 1.118061 -0.870619
C 4.422680 1.003392 -0.827607
C 5.045029 0.088531 0.029928
C 4.266436 -0.738775 0.850048
C 2.861574 -0.672572 0.827336
C 2.366262 2.112541 -1.826386
C 2.536329 1.642981 -3.290057
C 2.040773 -1.593238 1.726024
C 2.441213 -3.073564 1.548713
C -3.116267 -1.192687 0.726477
C -4.372297 -0.637106 1.429505

C -3.507259 -2.310121 -0.265955
C -2.156566 -1.787500 1.785373
C 2.161112 -1.169654 3.208454
C 2.920223 3.543272 -1.644264
C -4.103846 0.498295 -2.192437
C -4.122626 2.221994 -0.337040
H -0.196087 0.111778 -2.454082
H -3.975416 -3.132699 0.302328
H -4.228465 -1.965476 -1.020338
H -2.610699 -2.706162 -0.776164
H -4.797742 -1.428428 2.070937
H -4.133974 0.228075 2.068386
H -5.146049 -0.345243 0.704037
H -2.684527 -2.603493 2.308980
H -1.256227 -2.205763 1.301775
H -1.847424 -1.030491 2.522047
H 4.752783 -1.456811 1.513833
H 6.134876 0.016007 0.056192
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H 0.987680 -1.516266 1.423805
H 1.541641 -1.824937 3.844092
H 3.206661 -1.247203 3.551207
H 1.830515 -0.130122 3.354246
H 1.775640 -3.714945 2.149857
H 2.347841 -3.363459 0.487712
H 3.478767 -3.257080 1.874929
H 1.288835 2.135933 -1.608449
H 2.044749 2.350289 -3.979484
H 3.604988 1.585971 -3.556186
H 2.091075 0.646419 -3.433441
H 2.383122 4.243622 -2.305510
H 2.805561 3.884911 -0.603229
H 3.990803 3.590761 -1.902525
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H -4.899196 1.660701 0.197058
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H -3.504013 -0.215724 -2.779164
H -4.891682 -0.055711 -1.661448
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H -1.564060 2.745907 -1.351640
H -1.673259 1.637374 -2.742310
H -2.502728 2.091441 2.599759
H 1.810908 1.854576 2.151322
H 0.955365 4.216980 2.029019
H 0.734974 3.620163 0.364583
H -1.650819 3.830386 0.666329
H -1.384043 4.353887 2.349557
H -0.159179 2.628777 3.852452
H -0.304743 0.864176 3.494127
Pd 0.110771 -2.869665 -1.035635

64-Pd
C -0.092993 0.063144 3.476936
C -0.709553 -0.409170 2.297748
C -2.097300 -0.704271 2.365710

C -2.833164 -0.493836 3.539369
C -2.199246 -0.002719 4.693706
C -0.823178 0.266713 4.660334
Si 0.117182 -0.882135 0.645877
P 2.224518 0.179897 0.168536
C 2.959742 1.576824 1.260313
C 1.754918 2.494502 1.590643
C 1.597335 0.899821 -1.319781
C 0.213875 0.882723 -1.460388
C -0.123465 1.636376 -2.738503
C 0.204913 3.152495 -2.481551
C 1.769048 3.179023 -2.399564
C 2.146175 1.659513 -2.534902
C 1.101016 1.223247 -3.607478
N -0.647325 0.309904 -0.581509
C -2.072829 0.402728 -0.741258
C -2.769134 1.470379 -0.115002
C -4.175445 1.460549 -0.146030
C -4.879084 0.443909 -0.801444
C -4.175810 -0.566197 -1.468550
C -2.768792 -0.609641 -1.453900
C -2.052564 2.659776 0.522526
C -2.325445 2.794094 2.037294
C -2.047335 -1.693177 -2.251873
C -2.561538 -3.109418 -1.915684
C 3.541724 -1.145736 -0.213648
C 4.936555 -0.530038 -0.464903
C 3.616405 -2.142181 0.965021
C 3.106106 -1.885967 -1.499727
C -2.178730 -1.421327 -3.769548
C -2.473478 3.970107 -0.190441
C 3.591423 1.019572 2.554948
C 4.013962 2.427849 0.508048
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H 3.951814 -1.653195 1.892759
H 2.633055 -2.615455 1.135859
H 5.604678 -1.331776 -0.823791
H 4.907418 0.257921 -1.233256
H 5.377964 -0.118150 0.453352
H 3.839549 -2.687808 -1.696260
H 2.107146 -2.338242 -1.382662
H 3.085910 -1.203328 -2.363397
H -4.723347 -1.338976 -2.011933
H -5.971659 0.449240 -0.809631
H -4.720172 2.267920 0.347894
H -0.980705 -1.670917 -1.985167
H -1.641534 -2.197257 -4.340809
H -3.237353 -1.436707 -4.078850
H -1.758348 -0.439931 -4.039217
H -1.965841 -3.858969 -2.462571
H -2.460827 -3.304763 -0.834747
H -3.618731 -3.238789 -2.204517
H -0.971437 2.520301 0.385401
H -1.835507 3.704703 2.422657
H -3.407891 2.885937 2.226714
H -1.949892 1.929317 2.595327

H -1.853895 4.811550 0.162754
H -2.373115 3.890475 -1.283489
H -3.526172 4.207734 0.034015
H 4.157653 3.372816 1.061307
H 4.987526 1.927758 0.445555
H 3.686701 2.679184 -0.508839
H 3.820428 1.859621 3.233611
H 2.927934 0.323014 3.086947
H 4.533079 0.491474 2.344809
H 2.110007 3.332060 2.215741
H 1.321833 2.909984 0.667944
H 0.959042 1.969381 2.134479
H 3.201707 1.474407 -2.778419
H -1.127761 1.451362 -3.136459
H -0.167088 3.761132 -3.320300
H -0.263147 3.516849 -1.560150
H 2.119803 3.621184 -1.457733
H 2.201758 3.758420 -3.231846
H 1.168496 1.799787 -4.546360
H 1.131793 0.144459 -3.820287
H -2.611539 -1.103698 1.489190
H -3.903415 -0.713747 3.551880
H -2.770559 0.158991 5.610711
H -0.313832 0.636332 5.554018
H 0.974822 0.278603 3.485032
Pd 0.116480 -3.011791 0.168872

65-Pd

C	-0.249993	2.728999	2.953282
C	-0.625746	1.208356	2.913244
C	-0.463363	0.721074	1.474152
C	0.910578	0.692555	1.213008
C	1.612930	1.178630	2.472160
C	1.277474	2.713997	2.588316
C	0.656123	0.590036	3.549529
N	1.469719	0.343499	0.032864
Si	0.310829	-0.340198	-1.271361
P	-1.464162	0.263746	0.131328
Si	-4.034745	0.203341	-0.097631
C	-4.891503	-0.433953	-1.660946
C	2.898482	0.250810	-0.095512
C	3.563308	-0.934594	0.308139
C	4.961398	-0.991838	0.161419
C	5.678574	0.081765	-0.382238
C	5.001924	1.240504	-0.782146
C	3.606123	1.349300	-0.641204
C	2.812655	-2.116084	0.915828
C	3.140822	-3.438759	0.190593
C	2.890205	2.622046	-1.086240
C	2.899410	2.741462	-2.627509
N	-2.738937	-0.818922	0.532682
C	-2.679985	-2.228422	0.988405
C	-1.325267	-2.546355	1.655342
N	-2.718268	1.358841	-0.358303
C	-2.592157	2.554993	-1.220668
C	-2.557645	2.152020	-2.714294

C	3.499926	3.884262	-0.436500
C	3.106455	-2.237415	2.429106
C	-5.322629	0.760775	1.173532
C	-3.826934	3.442885	-0.952535
C	-1.314143	3.346375	-0.867564
C	-3.814332	-2.431181	2.017175
C	-2.889661	-3.172115	-0.218015
H	0.288224	0.837518	-2.208430
H	5.490195	-1.894610	0.474450
H	6.763249	0.014570	-0.494597
H	5.560532	2.076872	-1.207887
H	1.735678	-1.943995	0.782233
H	2.532563	-3.074487	2.861594
H	4.178725	-2.429224	2.603351
H	2.832208	-1.315335	2.963745
H	2.524481	-4.254129	0.604255
H	2.922991	-3.342120	-0.886962
H	4.201278	-3.717152	0.311394
H	1.841430	2.552655	-0.764661
H	2.354229	3.646701	-2.944569
H	3.933830	2.810460	-3.003529
H	2.420927	1.863928	-3.088853
H	2.916767	4.775583	-0.722094
H	3.502300	3.803120	0.662009
H	4.539141	4.040166	-0.769161
H	-1.583534	0.959909	3.390525
H	2.680128	0.938675	2.537589
H	1.886510	3.163831	3.387766
H	1.495304	3.246202	1.651808
H	-0.851091	3.313993	2.244196
H	-0.408688	3.141326	3.963494
H	0.871990	0.972107	4.561991
H	0.643653	-0.510095	3.554614
H	-3.775689	4.358105	-1.563932
H	-4.756582	2.910694	-1.217620
H	-3.873326	3.723082	0.111172
H	-1.251625	4.242923	-1.504771
H	-1.332552	3.659124	0.186599
H	-0.412787	2.739416	-1.040223
H	-2.475864	3.046032	-3.355060
H	-1.693934	1.500698	-2.913017
H	-3.476513	1.609744	-2.985451
H	-3.823903	-3.475160	2.369661
H	-3.673494	-1.761230	2.880023
H	-4.797328	-2.216726	1.564143
H	-2.853706	-4.226750	0.104067
H	-3.867498	-2.984138	-0.690694
H	-2.094918	-2.994917	-0.964716
H	-1.352626	-3.577890	2.042103
H	-0.507690	-2.473344	0.918035
H	-1.122582	-1.854990	2.486983
H	-6.017443	-0.054696	1.437818
H	-4.826690	1.100695	2.096956
H	-5.926284	1.597555	0.781189
H	-5.576440	-1.268710	-1.430633
H	-5.491589	0.355665	-2.146574

H	-4.145811	-0.795602	-2.386845
Pd	0.436638	-2.466107	-1.726203

66-Pd

C	-0.296898	3.938849	-0.127737
C	-0.221337	3.020843	0.947042
C	-0.290465	3.534672	2.262711
C	-0.438029	4.909033	2.502083
C	-0.530498	5.804900	1.424976
C	-0.455896	5.309654	0.111312
C	-0.003081	1.564794	0.748345
C	-0.842985	0.713311	-0.284711
C	-1.789959	1.429945	-1.215619
C	-1.608468	1.413108	-2.612745
C	-2.516438	2.060824	-3.464210
C	-3.613539	2.757578	-2.930555
C	-3.785037	2.813910	-1.537686
C	-2.879710	2.156106	-0.692114
Si	1.106107	0.819191	-0.623887
N	1.798466	-0.629872	0.318429
C	3.246038	-0.695378	0.317552
C	3.901272	-1.631165	-0.520832
C	5.306628	-1.614856	-0.564387
C	6.045509	-0.708623	0.206845
C	5.380370	0.187524	1.050182
C	3.975272	0.208378	1.128009
C	3.125121	-2.612428	-1.393852
C	3.683101	-4.050937	-1.318978
C	3.291408	1.203714	2.062894
C	3.817953	1.088986	3.511402
C	1.096577	-1.520579	1.051078
C	-0.289840	-1.690347	1.170154
C	-0.498523	-2.852363	2.153441
C	-0.102165	-2.353875	3.588431
C	1.436537	-2.086795	3.442136
C	1.740498	-2.559270	1.975368
C	0.739591	-3.731636	1.824298
P	-1.532535	-0.823578	0.310484
N	-3.059493	-0.765900	1.093584
C	-3.491757	-0.199205	2.392519
C	-3.715121	-1.357595	3.394181
Si	-3.927831	-1.620698	-0.193387
C	-4.647144	-3.294240	0.332283
N	-2.327422	-1.665361	-0.950127
C	-1.760665	-2.577632	-1.973598
C	-0.410647	-2.056715	-2.497125
C	-5.219206	-0.637565	-1.153146
C	3.085998	-2.103528	-2.852432
C	3.445151	2.649843	1.536127
C	-1.569948	-3.989769	-1.372357
C	-2.768321	-2.634075	-3.141546
C	-2.441564	0.778536	2.952977
C	-4.827260	0.550121	2.184709
H	5.825989	-2.319144	-1.216861
H	7.136679	-0.706437	0.153804
H	5.953829	0.888460	1.659917

H	2.092195	-2.656753	-1.027889
H	3.036508	-4.729810	-1.899312
H	4.698780	-4.115450	-1.741373
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H	2.495529	-2.787995	-3.484781
H	2.636022	-1.095418	-2.893319
H	4.109130	-2.045033	-3.260534
H	2.219160	0.973922	2.085042
H	2.867345	3.347095	2.163862
H	4.506313	2.951591	1.553621
H	3.078839	2.727446	0.500331
H	3.255640	1.773756	4.167808
H	3.709369	0.062329	3.897314
H	4.883307	1.364922	3.572010
H	-1.483442	-3.334286	2.095926
H	2.797691	-2.758878	1.773731
H	2.020187	-2.689000	4.155314
H	1.703179	-1.030417	3.587440
H	-0.657071	-1.456285	3.887720
H	-0.297997	-3.140312	4.335783
H	0.913256	-4.536502	2.558248
H	0.724586	-4.149394	0.807483
H	-5.160141	0.997279	3.135008
H	-4.714667	1.344134	1.433171
H	-5.613733	-0.144004	1.843668
H	-4.064774	-0.966778	4.364256
H	-4.474507	-2.055044	3.006273
H	-2.781717	-1.914993	3.551813
H	-2.768593	1.138458	3.940825
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H	-2.298951	1.645437	2.295553
H	-2.380956	-3.286345	-3.940450
H	-3.735953	-3.047752	-2.808094
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H	-0.535503	-1.106900	-3.028777
H	0.300659	-1.900667	-1.677014
H	-1.133918	-4.673661	-2.119349
H	-0.896617	-3.934755	-0.506102
H	-2.534253	-4.404202	-1.040830
H	-4.938104	-3.900859	-0.542959
H	-3.921193	-3.873290	0.924679
H	-5.555332	-3.154950	0.945193
H	-5.558290	-1.206359	-2.036521
H	-6.110061	-0.422546	-0.538736
H	-4.795381	0.317481	-1.497628
H	-0.714035	0.936459	-3.015852
H	-2.356483	2.035531	-4.544930
H	-4.316803	3.268337	-3.592502
H	-4.618905	3.374603	-1.108473
H	-3.002556	2.219646	0.387092
H	-0.219746	2.840461	3.104725
H	-0.484943	5.277628	3.530115
H	-0.651300	6.875479	1.605796
H	-0.512325	5.997767	-0.735855
H	-0.212376	3.569228	-1.150176

H	0.096170	1.040254	1.706405
Pd	2.106434	1.593753	-2.381116

67-Pd

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C 2.287450 -3.053192 1.670011
C 2.091350 -4.447449 1.636474
C 2.000021 -5.141109 0.424826
C 2.144420 -4.445299 -0.782938
N 2.464575 -0.910193 0.415358
C 3.735265 -0.377742 0.199885
C 4.099684 0.856800 -0.292353
C 5.642776 0.865517 -0.272126
C 6.157394 -0.121381 -1.385224
C 5.730988 -1.519336 -0.824897
C 5.019708 -1.153863 0.520740
C 5.916706 0.017652 1.000301
P 2.899918 2.119572 -0.789009
C 3.219954 3.578600 0.440221
C 1.939344 4.445702 0.467703
C 2.457568 -2.370280 3.028747
C 3.752507 -2.848201 3.732096
C 2.479233 -2.318552 -2.139348
C 3.250678 -3.124556 -3.208823
Si 1.008973 0.116221 0.907989
Si -1.265691 -0.153593 -0.341975
P -3.148319 -1.271028 -1.334431
C -3.357934 -0.905063 -3.198099
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C 2.572829 3.863765 -2.992058

C 4.927151 3.004193 -2.814681
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C 1.258316 -2.621382 3.969533
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68-Pd
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C 4.510208 1.212604 -0.624657
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C -1.299074 0.000165 2.409933
C -2.424832 -0.000005 3.178484
C 0.032457 0.000376 3.010458
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C -3.505627 -3.527212 1.141905
C 3.501146 -3.560312 1.051367
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69-Pd
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70-Pd
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C 3.597025 3.093566 -0.406371

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C 0.436021 -2.900294 2.828275
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H 0.827838 -3.915215 2.662147
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71-Pd
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C 3.039678 1.681270 -0.425230
C 4.321980 1.846326 -0.979527
C 5.221235 0.776526 -1.052200
C 4.836058 -0.485156 -0.585446
N 1.382729 0.241198 0.685481
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C -2.483012 0.753940 2.836126
C 2.088372 2.876006 -0.377672
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72-Pd
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C -4.880794 -0.359534 -0.534538
C -5.233755 0.909991 -1.002398
C -4.288568 1.941658 -0.974913
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73-Pd
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74-Pd
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75-Pd
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C 2.676648 0.406924 0.078546
C 3.016623 1.708382 -0.370878
C 4.303910 1.912607 -0.899541
C 5.223775 0.862314 -0.997661
C 4.857247 -0.418818 -0.573273
C 3.583685 -0.677309 -0.030197
C 2.048432 2.888676 -0.297348
C 1.826166 3.506153 -1.695855
C 3.252424 -2.101740 0.411727
C 3.349852 -3.076872 -0.784621
C 4.180987 -2.587477 1.550171
C 2.544033 3.971927 0.689307
C -4.178421 -2.581997 1.560181
C -2.536858 3.974911 0.675779
H 2.228952 0.748238 3.910113
H 5.567334 -1.243761 -0.658760
H 6.219519 1.040856 -1.410028
H 4.582059 2.911996 -1.239989
H 2.210041 -2.129900 0.762632
H 3.907848 -3.615516 1.840191
H 5.233254 -2.595118 1.220867
H 4.112810 -1.952017 2.447061
H 3.052445 -4.089366 -0.464166
H 2.675186 -2.753506 -1.593838
H 4.380880 -3.127162 -1.174561
H 1.078220 2.519288 0.056876
H 1.828666 4.810963 0.717824
H 2.649538 3.578553 1.712688
H 3.523306 4.368053 0.373819
H 1.122009 4.350294 -1.624416
H 2.771829 3.886845 -2.115381
H 1.405464 2.754889 -2.376879
H -4.582113 2.910444 -1.245835
H -6.221503 1.040130 -1.405815
H -5.569236 -1.242643 -0.649072
H -2.209249 -2.126899 0.767070
H -3.053854 -4.088532 -0.453614
H -4.385024 -3.128754 -1.162133
H -2.680938 -2.754961 -1.587517
H -3.905970 -3.610077 1.850716
H -4.106510 -1.945614 2.456108
H -5.231665 -2.588485 1.233994
H -1.075236 2.518271 0.042797
H -1.820835 4.813571 0.698298
H -3.517235 4.370551 0.363100
H -2.638149 3.585137 1.700982
H -1.121009 4.342881 -1.644623
H -1.411885 2.746019 -2.390821
H -2.774096 3.882424 -2.127452
H -2.228688 0.755568 3.908200
H -2.939735 1.647024 2.527390
H -3.247961 -0.078166 2.689124
H -0.000316 0.523677 3.741227
H 3.245208 -0.090432 2.691923

H 2.945373 1.636275 2.529834
H 0.002195 0.237248 -2.493978
Pd -0.002064 -2.555830 -0.914754

76-Pd
C 3.761013 -0.609559 -0.069041
C 2.831930 0.407153 -0.398565
C 3.046842 1.767347 -0.045100
C 4.247567 2.087930 0.613733
C 5.190430 1.102466 0.932603
C 4.939316 -0.230946 0.603011
N 1.628386 0.075884 -1.143705
Si 0.160845 -0.647828 -0.236979
O -0.044069 0.697469 0.935391
S 0.092526 0.635844 2.533483
C -1.723574 0.293403 2.977304
F -2.491061 1.325481 2.591531
C 2.023931 2.861495 -0.367949
C 2.017845 4.001698 0.673194
C 3.546285 -2.088269 -0.382173
C 3.425831 -2.894763 0.933419
C 1.665273 0.098005 -2.491967
C 2.996696 0.250959 -3.196631
C 0.497905 -0.014719 -3.273487
C -0.819179 0.062377 -2.780399
C -1.953098 0.244908 -3.763795
N -1.097282 -0.002645 -1.462517
C -2.438569 0.279763 -0.985804
C -3.354186 -0.782835 -0.774589
C -4.627245 -0.461010 -0.266346
C -4.990033 0.860141 0.012539
C -4.076621 1.893033 -0.223676
C -2.787781 1.629246 -0.719732
C -3.050786 -2.242105 -1.114757
C -3.206937 -3.164001 0.116112
C -1.841997 2.803780 -0.974415
C -1.597228 3.632148 0.306802
C -2.392549 3.731932 -2.085476
C -3.974219 -2.754349 -2.247947
O 0.375138 1.998522 3.003011
O 0.882077 -0.512019 2.991645
C 2.228745 3.452845 -1.783985
C 4.686456 -2.676664 -1.246189
F -2.148839 -0.827882 2.371454
F -1.811759 0.141491 4.309561
H -1.574752 0.265576 -4.794524
H -5.342065 -1.267692 -0.094210
H -5.982896 1.085268 0.408227
H -4.358839 2.926281 -0.013794
H -2.003230 -2.318147 -1.442623
H -3.704947 -3.790991 -2.509034
H -5.027470 -2.747464 -1.922048
H -3.904001 -2.140849 -3.159613
H -2.954815 -4.199778 -0.165924
H -2.534010 -2.847668 0.926502
H -4.244294 -3.155523 0.491078

H -0.873676 2.410924 -1.312356
H -1.675187 4.546288 -2.279557
H -2.566062 3.195070 -3.031022
H -3.347673 4.185084 -1.773529
H -0.963302 4.500711 0.068385
H -2.548052 4.012370 0.713578
H -1.097921 3.040586 1.081738
H 4.443239 3.122059 0.896030
H 6.111872 1.376243 1.451236
H 5.662114 -1.004098 0.870597
H 2.595539 -2.207035 -0.923687
H 3.186489 -3.947063 0.703957
H 4.375712 -2.870334 1.494545
H 2.629494 -2.478864 1.569887
H 4.469365 -3.731961 -1.479373
H 4.816992 -2.134158 -2.196099
H 5.646571 -2.640094 -0.705917
H 1.031463 2.397504 -0.343034
H 1.525996 4.288390 -1.941482
H 3.254557 3.842015 -1.898422
H 2.045971 2.709111 -2.572313
H 1.177186 4.678610 0.460968
H 1.897980 3.606576 1.691240
H 2.942218 4.600853 0.623387
H 2.851547 0.365773 -4.279201
H 3.555381 1.114450 -2.809833
H 3.615518 -0.639115 -3.008230
H 0.622990 -0.020258 -4.353832
H -2.681775 -0.571545 -3.658547
H -2.498184 1.177561 -3.560249
Pd 0.145703 -2.713550 0.370634

77-Pd
C -2.893755 1.850728 -0.431743
C -2.652567 0.529269 0.025793
C -3.652271 -0.473505 -0.036193
C -4.916432 -0.113584 -0.542260
C -5.188665 1.190949 -0.961533
C -4.179786 2.160537 -0.908656
N -1.363327 0.227192 0.623282
Si -0.010572 -0.644751 -0.378245
S 0.084938 0.552799 -2.229289
C -3.424133 -1.920577 0.394938
C -3.466821 -2.850982 -0.840070
C -1.808297 2.926998 -0.404846
C -1.841506 3.821075 -1.662882
C -1.248248 0.320603 1.964511
C -2.473090 0.625811 2.802459
C -0.013826 0.155713 2.627393
C 1.248260 0.161879 2.005131
C 2.485651 0.258995 2.872623
N 1.383891 0.095035 0.664300
C 2.673136 0.407790 0.080915
C 2.980399 1.770155 -0.169291
C 4.235236 2.077204 -0.722664
C 5.156632 1.069944 -1.033851

C 4.834081 -0.265546 -0.774475
C 3.597563 -0.625506 -0.203952
C 2.014841 2.906453 0.165131
C 1.735265 3.796026 -1.065941
C 3.328476 -2.096200 0.102899
C 3.259041 -2.924708 -1.199553
C 4.399992 -2.685061 1.050546
C 2.548278 3.776742 1.328706
C -4.460362 -2.403001 1.437545
C -1.884870 3.791064 0.875535
H 2.212136 0.341949 3.933181
H 5.553044 -1.053564 -1.007288
H 6.123565 1.326953 -1.472294
H 4.487469 3.121664 -0.915658
H 2.345032 -2.184720 0.590582
H 4.136034 -3.722961 1.311754
H 5.391901 -2.697732 0.569430
H 4.487549 -2.103951 1.982985
H 3.078924 -3.985930 -0.958546
H 2.428846 -2.571333 -1.831002
H 4.203994 -2.850528 -1.764621
H 1.061012 2.468925 0.488983
H 1.832664 4.585652 1.551644
H 2.695111 3.187327 2.246754
H 3.513292 4.236107 1.058167
H 1.024315 4.592226 -0.793818
H 2.660039 4.278341 -1.421624
H 1.310823 3.206348 -1.890596
H -4.392009 3.173456 -1.252323
H -6.179664 1.451794 -1.339868
H -5.694570 -0.876828 -0.600693
H -2.416444 -2.011341 0.829082
H -3.274720 -3.892053 -0.529699
H -4.455643 -2.808179 -1.328372
H -2.691974 -2.558257 -1.565825
H -4.206933 -3.425336 1.762367
H -4.494001 -1.757592 2.329589
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H -0.836684 2.419083 -0.391527
H -1.112725 4.578153 0.844866
H -2.871218 4.277359 0.958723
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H -0.030094 0.179893 3.714760
H 3.105612 -0.639218 2.726741
H 3.108035 1.119483 2.588999
H 0.072336 -0.544170 -3.017029
Pd -0.104068 -2.812479 -0.478125

78-Pd

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C -2.654988 0.510809 0.023612
C -3.642522 -0.504066 -0.046836
C -4.906092 -0.159443 -0.564102
C -5.190724 1.142317 -0.984565
C -4.194880 2.123978 -0.920064
N -1.365798 0.221170 0.628909
Si -0.005085 -0.644826 -0.358709
Cl 0.097567 0.568255 -2.126232
C -3.403394 -1.947685 0.389766
C -3.439940 -2.884524 -0.840762
C -1.844180 2.927368 -0.393323
C -1.829566 3.764079 -1.691328
C -1.248729 0.329792 1.968852
C -2.476961 0.631311 2.802533
C -0.012999 0.180463 2.633245
C 1.249969 0.180490 2.012476
C 2.487199 0.285809 2.878805
N 1.389154 0.096191 0.672937
C 2.674797 0.406566 0.079885
C 2.978893 1.767722 -0.182392
C 4.228698 2.069566 -0.750275
C 5.146745 1.059853 -1.063224
C 4.826693 -0.273851 -0.791999
C 3.595386 -0.629509 -0.207921
C 2.019140 2.907820 0.156003
C 1.725676 3.789287 -1.077453
C 3.328307 -2.098326 0.109296
C 3.257348 -2.935403 -1.187802
C 4.402002 -2.677567 1.060265
C 2.569914 3.785297 1.306298
C -4.435612 -2.430775 1.435979
C -2.018262 3.846371 0.838354
H 3.100668 -0.619818 2.750444
H 5.542906 -1.063644 -1.026945
H 6.109323 1.313615 -1.512905
H 4.479500 3.112468 -0.952969
H 2.346498 -2.184250 0.600558
H 4.143663 -3.715731 1.326042
H 5.394272 -2.686682 0.579938
H 4.484967 -2.091344 1.989983
H 3.066430 -3.993172 -0.939611
H 2.436013 -2.577552 -1.828539
H 4.206288 -2.875265 -1.747713
H 1.068385 2.473597 0.491752
H 1.857764 4.595898 1.534102
H 2.730516 3.202802 2.226526
H 3.530790 4.243044 1.018773
H 1.025063 4.592956 -0.800007
H 2.647304 4.261841 -1.453827
H 1.279517 3.194031 -1.885578
H -4.416320 3.136141 -1.260730
H -6.181512 1.391201 -1.371347
H -5.674089 -0.932260 -0.629726
H -2.395388 -2.028575 0.824886
H -3.231900 -3.921357 -0.526330

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H -2.675553 -2.583596 -1.574422
H -4.179483 -3.452054 1.762079
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H -0.865418 2.442208 -0.310449
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H -3.017369 4.313575 0.838807
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H -0.985345 4.468567 -1.667240
H -1.718047 3.113505 -2.571079
H -2.753190 4.354684 -1.804328
H -2.203734 0.770120 3.857192
H -2.990070 1.532301 2.436833
H -3.198841 -0.194364 2.721995
H -0.030005 0.216034 3.720234
H 3.115677 1.136023 2.578516
H 2.213959 0.391145 3.937385
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79-Pd
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C 2.383033 1.409935 0.849064
C 3.005992 2.312041 -0.051668
C 4.398793 2.490892 0.051336
C 5.151878 1.809666 1.011715
C 4.518729 0.909153 1.875069
N 0.937335 1.259511 0.825127
Si 0.151121 0.146323 -0.449855
O 0.993885 -1.335900 0.107028
S 1.400338 -2.629186 -0.748855
O 0.415867 -2.948507 -1.788440
C 2.254057 3.088384 -1.131481
C 2.753037 2.669539 -2.534774
C 2.502037 -0.345493 2.750032
C 3.295375 -1.672047 2.757573
C 0.184545 2.097251 1.574930
C 0.864553 3.213061 2.339445
C -1.212234 1.982500 1.661332
C -1.987822 0.888989 1.212203
C -3.458280 0.898473 1.509482
Si -4.331026 2.344936 0.531504
C -4.082351 3.972291 1.495634
N -1.436068 -0.108981 0.487931
C -2.043941 -1.425757 0.441590
C -1.839141 -2.275002 1.561682
C -2.366707 -3.576376 1.511791
C -3.057659 -4.035173 0.383847
C -3.245202 -3.182035 -0.706667
C -2.750825 -1.863459 -0.701996
C -1.096671 -1.813328 2.813796
C -0.018792 -2.825042 3.258128
C -3.047886 -0.964892 -1.896614
C -2.455188 -1.532771 -3.204630
C -4.574218 -0.762984 -2.040609
C -2.091949 -1.543265 3.966757

C 2.972276 -1.989897 -1.628643
F 3.686706 -3.056260 -2.026290
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F 2.653523 -1.246403 -2.700850
F 3.707164 -1.249739 -0.779117
C 2.402531 4.619336 -0.967435
C 2.379498 0.205230 4.189916
C -3.580220 2.523820 -1.205068
C -6.191992 1.941346 0.479562
H -3.785803 -3.535349 -1.586530
H -3.446422 -5.055417 0.356381
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H -2.576704 0.012811 -1.726485
H -4.792470 -0.073084 -2.872654
H -5.076072 -1.720781 -2.254250
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H -2.667212 -0.839565 -4.036657
H -1.366325 -1.654874 -3.108416
H -2.901578 -2.511158 -3.450322
H -0.586352 -0.868351 2.588002
H -1.553886 -1.169099 4.854011
H -2.849301 -0.799239 3.675472
H -2.615068 -2.472588 4.247138
H 0.552179 -2.405068 4.101702
H -0.474041 -3.769156 3.598940
H 0.673728 -3.048945 2.435975
H 5.108817 0.365337 2.614017
H 6.229954 1.971226 1.081559
H 4.891040 3.181318 -0.636258
H 1.186062 2.829297 -1.082089
H 2.151454 3.174339 -3.309426
H 3.809834 2.951960 -2.678671
H 2.654620 1.580891 -2.667477
H 1.831437 5.134229 -1.757463
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H 1.493570 -0.569672 2.387907
H 1.966632 -0.572181 4.854210
H 3.368013 0.500190 4.579746
H 1.713407 1.080545 4.239333
H 2.757918 -2.420506 3.357270
H 3.413174 -2.065530 1.740334
H 4.294492 -1.537167 3.203263
H 0.130305 3.789351 2.918332
H 1.630859 2.813528 3.018924
H 1.388927 3.884682 1.644532
H -1.734510 2.748364 2.228252
H -3.924427 -0.063068 1.253724
H -3.633599 1.093358 2.580401
H -3.744090 3.547454 -1.585218
H -2.491639 2.336194 -1.199514
H -4.031504 1.823337 -1.922570
H -6.750109 2.746613 -0.029192
H -6.397635 1.001985 -0.059422
H -6.606178 1.842418 1.497993
H -4.748876 4.755302 1.093292

H -4.314670 3.860312 2.569058
H -3.048904 4.344736 1.406271
Pd 0.021283 0.730531 -2.519772

80-Pd
C 3.926152 -2.410886 -0.340881
C 2.972930 -1.522074 -0.873119
C 2.650291 -1.762418 -2.217321
C 3.210914 -2.799219 -2.982770
C 4.153506 -3.652522 -2.400098
C 4.514125 -3.458655 -1.058639
B 2.474931 -0.252309 0.074868
C 1.749660 -0.723444 1.506717
C 1.377543 0.274679 2.424267
C 0.508527 0.080513 3.503830
C -0.019421 -1.196330 3.728739
C 0.325794 -2.234575 2.859849
C 1.211538 -1.986047 1.797168
F 1.829570 1.542982 2.249492
F 0.149790 1.101936 4.314787
F -0.870390 -1.408014 4.757442
F -0.236667 -3.456493 3.020028
F 1.434614 -3.056810 0.984781
F 1.722165 -1.003846 -2.876633
F 2.846421 -2.982033 -4.270523
F 4.701359 -4.653215 -3.115294
F 5.415227 -4.280482 -0.483702
F 4.308002 -2.276911 0.952869
C 1.299532 0.747629 -0.648820
C -0.100009 0.256971 -0.563748
C -0.374562 -1.127027 -0.616473
C -1.602199 -1.743488 -0.415564
C -1.680798 -3.248782 -0.371164
N -1.139209 1.144938 -0.429677
C -0.941737 2.557977 -0.750149
C -0.879511 2.898808 -2.124350
C -0.851039 4.264816 -2.454183
C -0.881282 5.250109 -1.459718
C -0.910379 4.881285 -0.110265
C -0.928361 3.527974 0.278670
C -0.882367 1.857685 -3.244233
C -2.234273 1.888860 -3.996746
C -0.900790 3.164668 1.760944
C -2.275724 3.388255 2.433811
Si -2.866416 0.762894 -0.228275
N -2.742515 -1.011326 -0.199469
C -4.022024 -1.678396 -0.010762
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C -5.646832 -2.682774 1.458356
C -6.525934 -2.826543 0.376216
C -6.142370 -2.404611 -0.901542
C -4.881518 -1.819877 -1.124694
C -3.434857 -1.920208 2.480840
C -3.771211 -0.601010 3.217911
C -4.488415 -1.397114 -2.538935
C -5.462038 -0.339209 -3.103303

C 0.309926 2.051462 -4.209153
C 0.178932 3.972421 2.521800
C -4.409299 -2.625476 -3.476201
C -3.456094 -3.116972 3.456142
C 3.842219 0.667373 0.269989
C 4.606106 0.754066 1.446440
C 5.781471 1.514289 1.554352
C 6.253856 2.219974 0.441053
C 5.545298 2.146227 -0.764706
C 4.377498 1.372908 -0.822427
F 4.241177 0.084323 2.566407
F 6.464930 1.569057 2.716548
F 7.379576 2.954661 0.525608
F 5.997123 2.808014 -1.851051
F 3.768547 1.318811 -2.043164
H -0.810043 4.554256 -3.505614
H -0.866570 6.306196 -1.737066
H -0.904599 5.650975 0.662459
H -0.770738 0.853150 -2.816845
H 0.317525 1.241523 -4.955565
H 0.238405 3.011419 -4.745094
H 1.266293 2.028796 -3.664385
H -2.254082 1.112832 -4.780112
H -3.074716 1.715757 -3.302802
H -2.387589 2.869603 -4.475776
H -0.644333 2.100222 1.850320
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H -5.145576 -0.034141 -4.113673
H -6.486585 -0.739542 -3.166544
H -5.474685 0.552636 -2.452179
H -4.091093 -2.313060 -4.483879
H -3.689962 -3.369887 -3.099012
H -5.393224 -3.114056 -3.561298
H -2.404470 -1.831963 2.107769
H -2.664258 -2.991266 4.204677
H -4.420374 -3.185921 3.984532
H -3.284798 -4.065590 2.923266
H -3.042721 -0.422986 4.022523
H -3.757089 0.258322 2.526284
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H -0.739103 -3.686589 -0.724422
H -1.841195 -3.577726 0.668937
H -2.523843 -3.623556 -0.970290
H 0.475119 -1.781715 -0.754467
H 1.548935 0.870410 -1.709534
H 1.346894 1.753547 -0.209383
Pd -4.591320 2.012920 -0.287737

81-Pd
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C 3.191721 -0.133728 -0.000749
C 3.665241 -0.764665 -1.167241
C 4.266073 0.047030 -2.147954
C 4.377145 1.430729 -1.970544
C 3.873080 2.033943 -0.809898
N 2.595620 -0.930875 1.039643
C 1.247412 -1.233488 1.097253
N 1.082425 -1.758861 2.370761
C 2.287966 -1.785497 3.073394
C 3.230549 -1.261065 2.238332
C -0.184670 -2.356554 2.741570
N -1.263310 -1.437694 2.436095
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C -4.564350 -0.024529 -2.024442
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C 4.903038 -2.952050 -1.459903
C 2.721351 1.935684 1.457240
C 3.892406 2.369165 2.370361
C 2.705560 -2.536025 -2.688533
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C -3.037491 2.948507 1.855013
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82-Pd
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C 2.445463 0.044516 0.539999
C 3.031141 1.291936 0.235329
C 4.362800 1.288781 -0.218286
C 5.073105 0.089886 -0.360029
C 4.461102 -1.133077 -0.052769
C 3.132147 -1.182473 0.404877
C 2.254289 2.601305 0.337850
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C 2.438716 -2.520032 0.653702
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C -2.253539 -2.601096 0.337420
C -1.972049 -3.163802 -1.074227
C -2.439905 2.520199 0.652962
C -1.995126 3.128564 -0.698377
C -2.986449 -3.637080 1.218667
C -3.317162 3.511499 1.447624
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H 1.404188 0.027322 3.132658

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H -6.106258 -0.108594 -0.715685
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83-Pd
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C 2.855602 -3.137386 -1.565566
C 2.208290 -3.404604 -0.346665
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C 1.428993 2.403361 0.252807
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84-Pd
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