Supplementary material

Ground States

Complex 3a E=-243.46319 a.u.

Pd	-0.1102	-0.4349	0.3490
Si	0.5934	-1.2859	2.3564
Cl	1.9572	-2.8880	2.0469
Cl	-0.8195	-2.0898	3.7102
Cl	1.6989	0.0667	3.5701
P	-0.8934	-0.2713	-1.8658
C	1.0661	2.5669	0.3716
C	2.0400	3.3402	-0.2825
C	2.7281	2.4501	-1.0901
C	2.4742	-0.0310	-1.6035
C	1.7519	-0.2200	-2.9267
C	0.4326	-0.3379	-3.1372
N	1.1460	1.2829	-0.0114
N	2.1709	1.2228	-0.9051
H	2.2206	4.4008	-0.1761
H	3.5616	2.5937	-1.7677
H	-0.9787	-1.6771	0.6722
H	-1.6000	0.8840	-2.3156
H	0.0913	-0.4914	-4.1621
H	0.3252	2.8682	1.1028
H	2.4056	-0.2953	-3.7998
H	3.5580	-0.0585	-1.7597
H	-1.7920	-1.2129	-2.4326
H	2.2205	-0.8440	-0.9052

Complex 3b E=-243.46808 a.u.

Pd	-0.1529	-0.5280	0.3023
Si	-1.4107	-2.1919	1.1348
Cl	-2.9507	-2.8800	-0.1911
Cl	-2.5327	-1.8221	2.8898
Cl	-0.3394	-3.9626	1.5577
P	-0.7433	-0.5933	-1.9560
C	0.4116	0.0483	-3.2326
C	1.7086	0.3005	-3.0136
C	2.4679	0.1018	-1.7171
C	1.3107	2.2869	0.8383
C	2.4008	3.0666	0.4174

C	2.9934	2.3371	-0.6007
N	2.2710	1.1948	-0.7553
N	1.2314	1.1520	0.1229
H	0.0896	-0.6956	1.8649
H	3.8676	2.5374	-1.2096
H	2.7322	4.0212	0.8058
H	0.5954	2.4700	1.6317
H	2.1650	-0.8188	-1.1985
H	-1.9139	0.1198	-2.3304
H	0.0021	0.2397	-4.2263
H	2.2967	0.6932	-3.8472
H	3.5428	0.0361	-1.9233
H	-1.1121	-1.8272	-2.5525

Complex 4a E=-293.85487 a.u.

Pd	0.0076	0.0292	0.0239
Si	1.0198	-0.0991	2.0747
Cl	-0.2108	-0.7154	3.6689
Cl	1.9679	1.6753	2.7107
Cl	2.6339	-1.4886	2.1866
P	1.1545	-1.7019	-1.0580
N	1.6844	1.6116	-3.8510
N	2.7414	1.8622	-3.0359
C	2.7842	-1.4765	-1.8649
C	3.4022	-0.3202	-2.1345
C	2.9237	1.0702	-1.8182
C	1.8326	2.4693	-4.8708
C	2.9855	3.2683	-4.7194
C	3.5482	2.8471	-3.5257
C	-1.5432	1.3041	-0.9861
C	-1.1963	0.4038	-1.9826
C	-1.9736	-0.7784	-2.4014
C	-3.0526	-1.3043	-1.6636
C	-3.7929	-2.3784	-2.1546
C	-3.4665	-2.9619	-3.3850
C	-1.6430	-1.3925	-3.6250
C	-2.3824	-2.4703	-4.1147
H	-0.4101	0.7075	-2.6812
H	0.4647	-2.3956	-2.0942
H	3.2715	-2.4068	-2.1648
H	1.0985	2.4827	-5.6696
H	4.3612	-0.3633	-2.6595
H	3.6658	1.5952	-1.2010
H	1.4492	-2.8201	-0.2388

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H         -0.4750      0.9755      1.2149
H          1.9740      1.0526     -1.2595
H          3.3484      4.0479     -5.3765
H          4.4347      3.1678     -2.9906
H         -2.4702      1.2105     -0.4213
H         -1.0827      2.2908     -0.9708
H         -3.3186     -0.8684     -0.6997
H         -4.6374     -2.7576     -1.5786
H         -4.0607     -3.7867     -3.7758
H         -0.8086     -0.9933     -4.2028
H         -2.1179     -2.9149     -5.0736

Complex 4b E=-293.84727 a.u.
Pd         0.0509      0.1466     -0.0517
Si        -1.4433      0.9465     -1.6179
Cl        -1.1193      2.8808     -2.3753
Cl        -3.4360      0.9209     -0.9216
Cl        -1.5887     -0.2329     -3.3732
P          1.0915     -1.6089     -1.2114
N          2.3054      1.4179     -4.1990
N          3.0421      1.8389     -3.1407
C          1.0951     -0.5892      1.9487
C          0.2378      0.4799      2.1577
C          2.7802     -1.4825     -1.9132
C          3.4666     -0.3644     -2.1751
C          3.0410      1.0511     -1.9093
C          2.4912      2.3583     -5.1342
C          3.3469      3.3866     -4.6818
C          3.6847      3.0172     -3.3899
C          2.5694     -0.5427      1.9390
C          3.3023      0.6603      1.9426
C          4.6941      0.6460      2.0021
C          5.3907     -0.5669      2.0524
C          3.2851     -1.7542      1.9852
C          4.6790     -1.7679      2.0407
H         -0.8408      1.4558      0.1689
H          0.6762     -1.5935      2.0449
H          0.3888     -2.1182     -2.3338
H          3.2345     -2.4424     -2.1671
H          1.9998      2.2545     -6.0961
H          4.4478     -0.4668     -2.6480
H          3.7488      1.5308     -1.2187
H          1.2382     -2.8431     -0.5196
H          2.0392      1.0878     -1.4474
H          3.6723      4.2732     -5.2121
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H          4.3148      3.4912     -2.6456
H          0.6151      1.4861      2.3345
H         -0.7854      0.2998      2.4821
H          2.7797      1.6163      1.9111
H          5.2428      1.5875      2.0239
H          6.4782     -0.5727      2.1118
H          2.7349     -2.6965      1.9963
H          5.2099     -2.7183      2.0826

Complex 4c E=-293.84916 a.u.
Pd        -0.0096      0.0516     -0.2643
Si        -1.5584      1.0810     -1.6195
Cl        -1.1494      3.0976     -2.0547
Cl        -3.5523      1.0345     -0.9287
Cl        -1.7684      0.2040     -3.5416
P          1.1048     -1.3658     -1.7709
N          2.4773      1.3550     -4.0180
N          3.2192      1.8434     -2.9932
C          1.2039     -0.9738      1.4845
C          0.5801      0.1956      1.8932
C          2.9395     -1.3652     -1.8574
C          3.7098     -0.2697     -1.8296
C          3.2138      1.1474     -1.7047
C          2.6603      2.2336     -5.0127
C          3.5188      3.2876     -4.6316
C          3.8582      3.0042     -3.3193
C          0.7068     -2.3411      1.7349
C         -0.6501     -2.6301      1.9777
C         -1.0614     -3.9319      2.2558
C         -0.1294     -4.9743      2.3014
C          1.6298     -3.4025      1.7649
C          1.2180     -4.7044      2.0518
H         -0.9792      1.2113      0.2547
H          0.7582     -1.2525     -3.1401
H          3.4132     -2.3422     -1.9711
H          2.1605      2.0716     -5.9617
H          4.7911     -0.3906     -1.9378
H          3.8620      1.7223     -1.0312
H          0.8742     -2.7557     -1.6021
H          2.1881      1.1680     -1.2964
H          3.8398      4.1386     -5.2186
H          4.4818      3.5287     -2.6048
H          1.1449      1.1265      1.9281
H         -0.3288      0.1711      2.4926
H          2.2502     -0.9112      1.1757
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H         -1.3910     -1.8329      1.9273
H         -2.1160     -4.1367      2.4366
H         -0.4523     -5.9895      2.5281
H          2.6848     -3.1954      1.5789
H          1.9526     -5.5087      2.0799

Complex 4d E=-293.85206 a.u.
Pd         0.0523      0.0294      0.0561
Si         1.0812     -0.0554      2.1101
Cl        -0.1157     -0.7338      3.7032
Cl         1.9746      1.7307      2.7811
Cl         2.7306     -1.4076      2.1830
P          1.2043     -1.6721     -1.0547
N          1.8680      1.5387     -3.9108
N          2.8254      1.8795     -3.0096
C          2.8466     -1.4515     -1.8330
C          3.4657     -0.2930     -2.0867
C          2.9699      1.0941     -1.7832
C          2.0392      2.3992     -4.9256
C          3.1047      3.2919     -4.6826
C          3.5908      2.9230     -3.4385
C         -1.2129      0.3367     -1.8323
C         -1.6669      1.2682     -0.9138
C         -1.3611      2.7167     -0.8989
C         -0.4820      3.3202     -1.8154
C         -0.2366      4.6919     -1.7613
C         -0.8622      5.4864     -0.7960
C         -1.9980      3.5308      0.0552
C         -1.7498      4.9011      0.1104
H         -2.5040      0.9800     -0.2740
H          0.5397     -2.3511     -2.1150
H          3.3428     -2.3808     -2.1194
H          1.3826      2.3430     -5.7877
H          4.4394     -0.3336     -2.5844
H          3.6883      1.6234     -1.1425
H          1.4745     -2.8163     -0.2636
H         -0.3963      0.9239      1.3128
H          2.0025      1.0756     -1.2563
H          3.4650      4.0952     -5.3130
H          4.4028      3.3153     -2.8371
H         -0.5465      0.6115     -2.6515
H         -1.7362     -0.6138     -1.9324
H          0.0165      2.7183     -2.5763
H          0.4468      5.1440     -2.4794
H         -0.6593      6.5556     -0.7513
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H	-2.6831	3.0738	0.7710
H	-2.2438	5.5120	0.8655

Complex 4e E=-293.85094 a.u.

Pd	0.0307	-0.0112	0.0124
Si	0.9487	1.2324	1.7152
Cl	-0.3797	2.4425	2.8054
Cl	2.5585	2.4848	1.1697
Cl	1.8405	0.0517	3.2486
P	0.2991	-2.1642	0.8710
N	2.2188	-2.0936	-3.0002
N	3.3162	-1.8343	-2.2446
C	1.8846	-3.0718	0.7325
C	2.9615	-2.7227	0.0188
C	3.1496	-1.4934	-0.8306
C	2.7052	-2.4257	-4.2042
C	4.1155	-2.3896	-4.2257
C	4.4752	-2.0072	-2.9434
C	-0.8712	-0.9317	-1.8951
C	-1.0415	0.4376	-1.9862
C	-2.2836	1.1854	-1.6794
C	-3.4611	0.5467	-1.2557
C	-4.6062	1.2831	-0.9601
C	-4.6014	2.6745	-1.0883
C	-2.2965	2.5850	-1.8147
C	-3.4417	3.3226	-1.5206
H	-0.5789	-3.1989	0.4391
H	1.9185	-4.0059	1.2975
H	2.0211	-2.6733	-5.0095
H	3.8175	-3.4039	0.0332
H	4.0502	-0.9494	-0.5145
H	0.0643	-2.3167	2.2614
H	0.1244	1.5919	0.0062
H	2.2915	-0.8076	-0.7466
H	4.7776	-2.6007	-5.0563
H	5.4436	-1.8331	-2.4886
H	-0.2810	1.0069	-2.5248
H	-0.0173	-1.4136	-2.3753
H	-1.6907	-1.5804	-1.5871
H	-3.4854	-0.5383	-1.1570
H	-5.5084	0.7705	-0.6273
H	-5.4971	3.2481	-0.8541
H	-1.3879	3.0975	-2.1332
H	-3.4275	4.4069	-1.6232

Complex 5a E=-293.85523 a.u.

Pd	0.0281	-0.0607	-0.1024
Si	1.0274	-0.1054	2.0265
Cl	-0.2831	-0.5944	3.6249
Cl	1.8659	1.7677	2.6056
Cl	2.6623	-1.4547	2.3276
P	1.1912	-1.7779	-1.0101
N	1.6768	1.6165	-3.7305
N	2.7536	1.8430	-2.9342
C	2.8078	-1.5159	-1.8299
C	3.4235	-0.3542	-2.0796
C	2.9521	1.0304	-1.7333
C	1.8197	2.4800	-4.7462
C	2.9900	3.2572	-4.6123
C	3.5685	2.8160	-3.4334
C	-1.4460	1.5859	-0.8000
C	-1.1866	0.5316	-1.8011
C	-2.2103	-0.4397	-2.2122
C	-3.4501	-0.5909	-1.5554
C	-4.3941	-1.5129	-2.0035
C	-4.1277	-2.3137	-3.1178
C	-1.9635	-1.2535	-3.3407
C	-2.9067	-2.1760	-3.7864
H	-0.4599	0.7922	-2.5759
H	0.5306	-2.5554	-2.0048
H	3.2961	-2.4388	-2.1519
H	1.0683	2.5118	-5.5288
H	4.3797	-0.3877	-2.6101
H	3.6980	1.5436	-1.1120
H	1.5351	-2.8298	-0.1245
H	-0.9755	1.3665	0.3038
H	2.0091	1.0040	-1.1649
H	3.3528	4.0380	-5.2693
H	4.4729	3.1158	-2.9171
H	-2.4937	1.7181	-0.5058
H	-0.9793	2.5466	-1.0351
H	-3.6905	0.0255	-0.6895
H	-5.3461	-1.6035	-1.4797
H	-4.8684	-3.0335	-3.4614
H	-1.0208	-1.1353	-3.8769
H	-2.6938	-2.7820	-4.6671

Complex 5b E=-293.84380 a.u.

Pd	0.0904	-0.0543	-0.1153

Si	-1.4471	0.9731	-1.5784
Cl	-1.0435	2.9970	-2.0829
Cl	-3.3722	1.0573	-0.6693
Cl	-1.8553	0.0734	-3.4583
P	0.9524	-1.6343	-1.4776
N	2.2651	1.4485	-4.3595
N	2.9721	1.8447	-3.2725
C	1.0741	-0.5661	1.7496
C	0.1958	0.5708	2.1046
C	2.6754	-1.4887	-2.0695
C	3.3645	-0.3612	-2.2818
C	2.9131	1.0530	-2.0455
C	2.4759	2.4109	-5.2667
C	3.3161	3.4294	-4.7670
C	3.6149	3.0314	-3.4747
C	2.5422	-0.4676	1.7736
C	3.2373	0.7603	1.7385
C	4.6304	0.8002	1.7907
C	5.3729	-0.3817	1.8710
C	3.3107	-1.6496	1.8513
C	4.7020	-1.6084	1.8980
H	-0.4394	1.0468	1.1833
H	0.6918	-1.5499	2.0339
H	0.2487	-1.9321	-2.6729
H	3.1556	-2.4449	-2.2865
H	2.0041	2.3334	-6.2404
H	4.3786	-0.4581	-2.6785
H	3.5833	1.5370	-1.3211
H	0.9928	-2.9469	-0.9356
H	1.8896	1.0889	-1.6357
H	3.6529	4.3286	-5.2679
H	4.2128	3.4939	-2.6986
H	-0.6312	0.3150	2.7744
H	0.7176	1.4706	2.4463
H	2.6854	1.6993	1.6848
H	5.1396	1.7640	1.7855
H	6.4599	-0.3466	1.9271
H	2.7975	-2.6119	1.8912
H	5.2667	-2.5378	1.9693

Complex 5c E=-293.83749 a.u.

Pd	0.0360	-0.0687	-0.2518
Si	-1.5236	1.0405	-1.6231
Cl	-1.0949	3.0945	-1.9668
Cl	-3.4734	1.0780	-0.7665

Cl	-1.8914	0.2844	-3.5806
P	1.0520	-1.3513	-1.8105
N	2.4917	1.3661	-4.0900
N	3.2032	1.8610	-3.0475
C	1.0867	-0.7140	1.5352
C	0.4406	0.5581	1.9324
C	2.8833	-1.3466	-1.8966
C	3.6545	-0.2517	-1.8806
C	3.1605	1.1655	-1.7609
C	2.6988	2.2396	-5.0841
C	3.5434	3.2980	-4.6838
C	3.8484	3.0217	-3.3612
C	0.5973	-1.9977	2.0577
C	-0.7190	-2.1590	2.5436
C	-1.1403	-3.3698	3.0901
C	-0.2663	-4.4580	3.1597
C	1.4589	-3.1146	2.1149
C	1.0330	-4.3240	2.6591
H	-0.3690	0.9932	1.1389
H	0.6857	-1.1300	-3.1607
H	3.3522	-2.3270	-1.9987
H	2.2275	2.0686	-6.0465
H	4.7352	-0.3750	-1.9917
H	3.7931	1.7359	-1.0679
H	0.8033	-2.7438	-1.7222
H	2.1248	1.1880	-1.3797
H	3.8811	4.1464	-5.2659
H	4.4521	3.5524	-2.6340
H	-0.2212	0.4859	2.8037
H	1.1304	1.4008	2.0304
H	2.1645	-0.6705	1.3680
H	-1.4224	-1.3271	2.5010
H	-2.1559	-3.4619	3.4741
H	-0.5900	-5.3960	3.6083
H	2.4822	-3.0181	1.7477
H	1.7218	-5.1665	2.7090

Complex 5e E=-293.85551 a.u.

Pd	-0.3710	0.1040	-0.4197
Si	-0.0411	0.7207	1.8304
Cl	-1.7745	1.4208	2.8394
Cl	1.4104	2.2215	2.2550
Cl	0.6150	-0.8941	3.0704
P	1.4528	-1.2015	-0.5679
N	6.8877	-1.1244	-2.7097

N	5.6191	-0.6544	-2.5753
C	3.0423	-0.5452	0.0248
C	4.2559	-0.6545	-0.5361
C	4.6536	-1.4010	-1.7770
C	7.4975	-0.2236	-3.4924
C	6.6291	0.8290	-3.8582
C	5.4259	0.5203	-3.2463
C	-1.1840	-0.1683	-2.3417
C	-2.2334	0.6519	-1.6974
C	-3.5905	0.0413	-1.4293
C	-3.7340	-1.1840	-0.7624
C	-5.0018	-1.7332	-0.5572
C	-6.1410	-1.0605	-1.0119
C	-4.7372	0.7165	-1.8658
C	-6.0048	0.1675	-1.6621
H	1.7831	-1.7646	-1.8284
H	2.9466	0.0305	0.9471
H	8.5337	-0.3764	-3.7758
H	5.0932	-0.1666	-0.0284
H	3.7906	-1.6702	-2.4011
H	1.2964	-2.4034	0.1697
H	-1.8716	1.0289	-0.5631
H	5.1716	-2.3319	-1.5051
H	6.8505	1.6801	-4.4911
H	4.4677	1.0290	-3.2432
H	-2.3180	1.6556	-2.1342
H	-0.5616	0.3293	-3.0886
H	-1.4383	-1.2007	-2.5873
H	-2.8451	-1.7035	-0.3976
H	-5.1031	-2.6864	-0.0381
H	-7.1314	-1.4902	-0.8604
H	-4.6390	1.6699	-2.3865
H	-6.8859	0.7014	-2.0153

Complex 6a E=-293.86803 a.u.

Pd	-0.0241	-0.0787	0.1743
Si	1.3940	0.2188	1.9348
Cl	0.5050	-0.1559	3.8227
Cl	2.3040	2.1251	2.1333
Cl	3.0664	-1.0985	1.9817
P	1.0593	-1.8687	-0.8412
N	1.5017	1.4632	-3.7884
N	2.5993	1.6838	-3.0215
C	2.5948	-1.6786	-1.8269
C	3.2080	-0.5446	-2.1853

C	2.8202	0.8624	-1.8295
C	1.6032	2.3496	-4.7895
C	2.7656	3.1404	-4.6721
C	3.3839	2.6819	-3.5201
C	-2.2032	0.7206	0.1026
C	-1.2148	1.6427	0.6432
C	-1.4245	2.3251	1.9767
C	-3.2785	0.1684	0.8587
C	-4.0738	-0.8274	0.3231
C	-3.8201	-1.3635	-0.9586
C	-2.7803	-0.8534	-1.7199
C	-1.9792	0.1929	-1.2134
H	-0.7611	2.2964	-0.1158
H	0.3045	-2.6357	-1.7743
H	3.0263	-2.6251	-2.1576
H	0.8276	2.3872	-5.5479
H	4.1024	-0.6289	-2.8094
H	3.6243	1.3371	-1.2504
H	1.4399	-2.9467	-0.0067
H	-0.5648	2.9643	2.2206
H	1.9072	0.8877	-1.2135
H	3.1003	3.9390	-5.3214
H	4.2961	2.9872	-3.0227
H	-1.5549	1.6136	2.8011
H	-2.3214	2.9697	1.9414
H	-3.4872	0.5521	1.8568
H	-4.9118	-1.2063	0.9053
H	-4.4572	-2.1538	-1.3535
H	-1.2887	0.7000	-1.8886
H	-2.5934	-1.2314	-2.7254

Complex 6b E=-293.86549 a.u.

Pd	-0.0326	-0.3933	-0.1255
Si	-1.8900	0.4282	-1.1719
Cl	-2.0078	2.5413	-1.2575
Cl	-3.7457	-0.1683	-0.3383
Cl	-2.1217	-0.1382	-3.2094
P	1.1216	-1.1543	-1.9893
N	2.5345	1.5665	-4.3200
N	3.1849	2.0944	-3.2535
C	0.6271	-0.1805	2.0872
C	1.1176	-1.4957	1.8118
C	1.5786	0.7996	2.4915
C	-0.7745	0.1220	1.8057

C	-1.3535	1.4691	2.1733
C	2.9534	-1.1006	-2.0003
C	3.6752	0.0275	-1.9943
C	3.1016	1.4208	-1.9556
C	2.7926	2.4142	-5.3256
C	3.6062	3.4899	-4.9089
C	3.8396	3.2509	-3.5645
C	2.9146	0.4727	2.6508
C	3.3771	-0.8305	2.3860
C	2.4813	-1.8044	1.9676
H	-2.3866	1.5485	1.8179
H	-1.4603	-0.7105	1.9993
H	0.8108	-0.5806	-3.2445
H	3.4658	-2.0642	-2.0107
H	2.3842	2.2115	-6.3104
H	4.7650	-0.0442	-2.0356
H	3.6582	2.0411	-1.2403
H	0.9123	-2.5187	-2.3183
H	2.0495	1.4081	-1.6325
H	3.9699	4.3241	-5.4966
H	4.3969	3.8093	-2.8215
H	-1.3688	1.6016	3.2687
H	-0.7957	2.3078	1.7393
H	1.2337	1.8078	2.7126
H	3.6170	1.2322	2.9937
H	4.4288	-1.0740	2.5279
H	0.4034	-2.3004	1.6260
H	2.8246	-2.8220	1.7854

Complex 6c E=-293.86801 a.u.

Pd	0.1306	-0.3024	-0.0988
Si	-1.4671	0.8770	-1.2374
Cl	-0.9813	2.9024	-1.6325
Cl	-3.3556	0.9881	-0.2755
Cl	-1.9864	0.1163	-3.1453
P	0.9724	-1.7524	-1.7088
N	2.1509	1.3370	-4.3577
N	2.9128	1.7347	-3.3092
C	1.5605	-0.8669	1.9228
C	0.2074	-0.4702	2.1603
C	-0.2830	0.8156	1.6619
C	0.5500	2.0790	1.7683
C	2.7274	-1.6056	-2.2312
C	3.4202	-0.4665	-2.3580

C	2.9289	0.9297	-2.0877
C	2.3406	2.2813	-5.2886
C	3.2250	3.2878	-4.8419
C	3.5749	2.9018	-3.5585
C	2.0058	-2.1583	2.2692
C	1.1317	-3.0719	2.8387
C	-0.6715	-1.4491	2.7141
C	-0.2128	-2.7075	3.0582
H	0.1825	2.8519	1.0826
H	-1.3453	0.9821	1.8558
H	0.3176	-1.8784	-2.9612
H	3.2268	-2.5461	-2.4727
H	1.8294	2.1975	-6.2421
H	4.4526	-0.5298	-2.7140
H	3.6062	1.4378	-1.3871
H	0.9606	-3.1287	-1.3528
H	1.9196	0.9229	-1.6423
H	3.5655	4.1689	-5.3712
H	4.2217	3.3595	-2.8187
H	0.4908	2.4830	2.7931
H	1.6115	1.9160	1.5449
H	2.2902	-0.1267	1.5965
H	3.0487	-2.4251	2.1011
H	1.4774	-4.0649	3.1215
H	-1.7142	-1.1793	2.8796
H	-0.8993	-3.4264	3.5046

Complex 6d E=-293.86764 a.u.

Pd	0.0056	-0.2848	-0.0710
Si	-1.5394	0.8674	-1.3091
Cl	-1.4868	2.9833	-1.1416
Cl	-3.5378	0.3490	-0.8366
Cl	-1.4752	0.5821	-3.4081
P	0.8955	-1.7189	-1.6629
N	2.5733	1.2347	-4.4708
N	3.1007	1.6830	-3.3047
C	1.4870	-0.8095	1.8077
C	0.1549	-0.4672	2.2106
C	-0.4053	0.7930	1.7365
C	2.6830	-1.6249	-2.0783
C	3.3986	-0.5040	-2.2370
C	2.9067	0.9088	-2.0795
C	2.8878	2.1801	-5.3662
C	3.6128	3.2399	-4.7787

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C          3.7321      2.8848     -3.4456
C          2.0280     -2.0773      2.1056
C          1.2716     -3.0149      2.7903
C         -0.5971     -1.4625      2.9026
C         -0.0432     -2.6967      3.1910
C         -1.7523      1.2793      2.2153
H          0.3340      1.5973      1.6348
H          0.3122     -1.8071     -2.9527
H          3.1799     -2.5857     -2.2229
H          2.5816      2.0571     -6.3996
H          4.4499     -0.6008     -2.5237
H          3.4815      1.4193     -1.2932
H          0.8156     -3.0938     -1.3148
H          1.8442      0.9341     -1.7877
H          4.0025      4.1322     -5.2521
H          4.2020      3.3822     -2.6052
H          2.1444     -0.0273      1.4220
H          3.0530     -2.3040      1.8139
H          1.6922     -3.9891      3.0336
H         -1.6136     -1.2328      3.2173
H         -0.6295     -3.4364      3.7361
H         -2.0405      2.1933      1.6836
H         -2.5524      0.5457      2.0626
H         -1.7120      1.5201      3.2905

Complex 6e E=-293.86562 a.u.
Pd         0.1306     -0.3024     -0.0988
Si        -1.4671      0.8770     -1.2374
Cl        -0.9813      2.9024     -1.6325
Cl        -3.3556      0.9881     -0.2755
Cl        -1.9864      0.1163     -3.1453
P          0.9724     -1.7524     -1.7088
N          2.1509      1.3370     -4.3577
N          2.9128      1.7347     -3.3092
C          1.5605     -0.8669      1.9228
C          0.2074     -0.4702      2.1603
C         -0.2830      0.8156      1.6619
C          0.5500      2.0790      1.7683
C          2.7274     -1.6056     -2.2312
C          3.4202     -0.4665     -2.3580
C          2.9289      0.9297     -2.0877
C          2.3406      2.2813     -5.2886
C          3.2250      3.2878     -4.8419
C          3.5749      2.9018     -3.5585
C          2.0058     -2.1583      2.2692
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C	1.1317	-3.0719	2.8387
C	-0.6715	-1.4491	2.7141
C	-0.2128	-2.7075	3.0582
H	0.1825	2.8519	1.0826
H	-1.3453	0.9821	1.8558
H	0.3176	-1.8784	-2.9612
H	3.2268	-2.5461	-2.4727
H	1.8294	2.1975	-6.2421
H	4.4526	-0.5298	-2.7140
H	3.6062	1.4378	-1.3871
H	0.9606	-3.1287	-1.3528
H	1.9196	0.9229	-1.6423
H	3.5655	4.1689	-5.3712
H	4.2217	3.3595	-2.8187
H	0.4908	2.4830	2.7931
H	1.6115	1.9160	1.5449
H	2.2902	-0.1267	1.5965
H	3.0487	-2.4251	2.1011
H	1.4774	-4.0649	3.1215
H	-1.7142	-1.1793	2.8796
H	-0.8993	-3.4264	3.5046

Complex 8a E=-293.84642 a.u.

Pd	-0.2710	-0.5880	-0.3766
Si	0.1554	1.5531	2.5220
Cl	-0.4743	0.0335	3.7873
Cl	0.5006	3.2065	3.7450
Cl	2.0278	1.0394	1.7875
P	1.3081	-2.1195	-0.8332
N	1.3463	1.4699	-4.2231
N	2.3785	1.5905	-3.3499
C	2.4782	-1.9069	-2.2360
C	2.8943	-0.7408	-2.7492
C	2.5241	0.6304	-2.2571
C	1.5276	2.4695	-5.0977
C	2.6753	3.2324	-4.7949
C	3.2011	2.6339	-3.6606
C	-1.7314	0.9126	0.3705
C	-1.0701	2.0436	1.1615
C	-2.1492	3.0297	1.6799
C	-2.6721	0.0417	0.9979
C	-3.6156	-0.6621	0.2553
C	-3.6384	-0.5682	-1.1460
C	-2.6866	0.2072	-1.7994
C	-1.7365	0.9557	-1.0612

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H         -0.4161      2.5903      0.4615
H          0.9401     -3.4685     -1.0949
H          2.8434     -2.8313     -2.6880
H          0.8188      2.5991     -5.9082
H          3.5781     -0.7598     -3.6030
H          3.3023      1.0241     -1.5865
H          2.2323     -2.4348      0.2055
H         -1.7010      3.9278      2.1189
H          1.5817      0.5823     -1.6756
H          3.0639      4.0972     -5.3179
H          4.0743      2.8669     -3.0610
H         -2.7921      2.5590      2.4339
H         -2.7931      3.3366      0.8449
H         -2.6900     -0.0222      2.0850
H         -4.3435     -1.2857      0.7724
H         -4.3890     -1.1114     -1.7183
H         -1.1366      1.7030     -1.5830
H         -2.6811      0.2781     -2.8858

Complex 9a E=-293.85487 a.u.
Pd        -0.0371      0.0613     -0.0246
P          1.1615     -1.7010     -1.0493
N          1.6896      1.5952     -3.8503
N          2.7456      1.8498     -3.0354
C          2.7923     -1.4911     -1.8619
C          3.4095     -0.3360     -2.1399
C          2.9310      1.0548     -1.8210
C          1.8371      2.4522     -4.8710
C          2.9893      3.2531     -4.7211
C          3.5524      2.8336     -3.5272
C         -1.5693      1.3137     -1.0203
C         -1.1873      0.3897     -1.9902
C         -1.9685     -0.7911     -2.4117
C         -3.0492     -1.3119     -1.6740
C         -3.7872     -2.3893     -2.1604
C         -3.4606     -2.9767     -3.3882
C         -1.6406     -1.4046     -3.6357
C         -2.3799     -2.4844     -4.1222
Si        -0.5020      1.3040      1.8890
H         -0.4051      0.6941     -2.6923
H          0.4799     -2.4209     -2.0728
H          3.2743     -2.4235     -2.1645
H          1.1038      2.4619     -5.6706
H          4.3650     -0.3819     -2.6722
H          3.6740      1.5791     -1.2040
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H          1.4605     -2.8189     -0.2304
H          0.7487     -0.2102      1.3151
H          1.9814      1.0372     -1.2619
H          3.3572      4.0284     -5.3814
H          4.4426      3.1527     -2.9978
H         -2.5147      1.2192     -0.4856
H         -1.1360      2.3122     -1.0294
H         -3.3144     -0.8734     -0.7122
H         -4.6279     -2.7716     -1.5817
H         -4.0482     -3.8099     -3.7720
H         -0.8068     -1.0095     -4.2173
H         -2.1155     -2.9354     -5.0782
Cl        -2.5026      1.0022      2.5117
Cl        -0.3199      3.3864      1.5436
Cl         0.5647      1.0855      3.7003

Complex 9b E=-293.79113 a.u.
Pd         0.0072      0.1529     -0.2099
P          1.0754     -1.5989     -0.9610
N          1.6411      1.6631     -3.9067
N          2.7012      1.9135     -3.0987
C          2.6748     -1.4048     -1.8168
C          3.2974     -0.2704     -2.1588
C          2.8699      1.1412     -1.8686
C          1.7943      2.5070     -4.9372
C          2.9558      3.2963     -4.7993
C          3.5178      2.8836     -3.6021
C         -2.0322      1.7359     -2.0548
C         -1.1801      0.4333     -2.0381
C         -1.9657     -0.7646     -2.4632
C         -3.0888     -1.2440     -1.7565
C         -3.8392     -2.3215     -2.2295
C         -3.4858     -2.9665     -3.4207
C         -1.6268     -1.4312     -3.6594
C         -2.3735     -2.5127     -4.1333
Si        -2.4700      2.5588     -0.4526
H         -0.3766      0.5977     -2.7691
H          0.3856     -2.4266     -1.8960
H          3.1392     -2.3553     -2.0940
H          1.0560      2.5141     -5.7324
H          4.2311     -0.3535     -2.7231
H          3.6443      1.6471     -1.2751
H          1.4253     -2.5878     -0.0119
H          0.9779     -0.0341      1.0647
H          1.9263      1.1630     -1.2978
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H	3.3266	4.0641	-5.4652
H	4.4093	3.2023	-3.0752
H	-2.9840	1.5800	-2.5924
H	-1.4934	2.5260	-2.6051
H	-3.3801	-0.7589	-0.8229
H	-4.7172	-2.6514	-1.6719
H	-4.0860	-3.7930	-3.8019
H	-0.7886	-1.0535	-4.2466
H	-2.1030	-2.9752	-5.0825
Cl	-4.2097	1.9508	0.4975
Cl	-2.5543	4.6302	-0.6311
Cl	-0.8906	2.1334	0.9202

Complex 10a E=-243.40274 a.u.

Pd	2.880	0.067	-0.627
P	0.563	-0.379	-0.308
N	1.780	2.404	-2.214
N	2.315	2.103	-0.999
Si	5.079	-0.156	-1.273
H	3.376	-1.397	-0.481
C	-1.052	0.906	-3.847
C	-1.822	-0.186	-1.992
C	1.786	1.752	-4.566
H	0.946	4.155	-3.128
C	2.655	3.243	1.186
C	-0.159	0.545	1.136
C	-0.125	-2.046	0.172
H	1.610	5.306	-0.740
H	2.170	0.497	-2.872
C	-0.436	0.095	-1.754
C	0.057	0.770	-2.957
C	1.457	1.301	-3.151
C	2.268	3.230	-0.270
C	1.711	4.272	-1.026
C	1.405	3.715	-2.254
Cl	5.811	1.562	-2.299
Cl	6.482	-0.493	0.272
Cl	5.478	-1.680	-2.689
Fe	-0.733	-1.031	-3.443
C	-2.230	0.328	-3.268
C	0.580	-2.570	-3.443
C	0.534	-1.950	-4.734
C	-0.818	-2.010	-5.208
C	-1.606	-2.675	-4.213

C	-0.743	-3.023	-3.122
C	3.959	2.940	1.593
C	4.195	2.567	2.920
C	3.187	2.701	3.878
C	1.970	3.279	3.504
C	1.701	3.569	2.160
C	-1.313	1.329	1.035
C	-1.880	1.888	2.184
C	-1.271	1.705	3.429
C	-0.084	0.974	3.522
C	0.476	0.408	2.374
C	0.653	-3.189	-0.042
C	0.145	-4.461	0.237
C	-1.148	-4.599	0.748
C	-1.919	-3.461	0.996
C	-1.404	-2.190	0.723
H	-1.550	-5.586	0.954
H	0.753	-5.341	0.055
H	1.661	-3.095	-0.425
H	-2.010	-1.322	0.950
H	-2.921	-3.564	1.402
H	1.230	3.502	4.265
C	3.429	2.225	5.315
H	5.168	2.183	3.208
C	5.146	3.043	0.632
C	0.372	4.239	1.780
H	-2.795	2.468	2.109
H	-1.777	1.509	0.074
H	1.407	-0.146	2.443
H	0.402	0.845	4.484
H	-1.717	2.133	4.321
H	1.128	2.569	-4.895
H	2.828	2.107	-4.613
H	1.671	0.916	-5.270
H	1.383	-1.544	-5.275
H	1.468	-2.691	-2.834
H	-1.044	-3.544	-2.220
H	-2.672	-2.873	-4.270
H	-1.180	-1.620	-6.154
H	-1.021	1.368	-4.828
H	-2.483	-0.718	-1.320
H	-3.216	0.261	-3.717
H	-0.349	4.224	2.610
H	0.571	5.290	1.525
H	-0.089	3.740	0.917

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      H     2.485    2.126    5.873
      H     3.930    1.245    5.305
      H     4.073    2.953    5.829
      H     5.845    3.798    1.021
      H     5.665    2.081    0.584
      H     4.841    3.350   -0.379
      XX   -1.093    0.387   -2.759
      XX   -0.410   -2.449   -4.145

Complex 10b E=-243.41062 a.u.

      Pd    2.930   -0.544   -0.164
      P     0.631   -0.725    0.182
      N     1.970    1.934   -1.806
      N     2.535    1.579   -0.610
      Si    3.578   -2.591    0.501
      C    -0.254   -0.355   -1.337
      C     0.239    0.320   -2.540
      C     1.644    0.821   -2.734
      C     2.540    2.685    0.153
      C     1.972    3.760   -0.555
      C     1.602    3.247   -1.787
      C    -0.893    0.557   -3.380
      C    -1.669   -0.501   -1.508
      C     2.038    1.166   -4.161
      C     0.868    3.945   -2.880
      C     2.989    2.649    1.602
      C     0.242    0.700    1.307
      C    -0.443   -2.063    0.891
      H     4.476   -0.489   -0.523
      H     1.847    4.788   -0.243
      H     2.330    0.014   -2.398
      Cl    2.350   -3.321    2.097
      Cl    3.379   -4.078   -0.985
      Cl    5.497   -2.869    1.327
      Fe   -0.749   -1.398   -3.047
      C    -2.091    0.076   -2.752
      C     0.342   -3.097   -3.165
      C     0.357   -2.403   -4.419
      C    -0.999   -2.256   -4.860
      C    -1.851   -2.868   -3.882
      C    -1.023   -3.390   -2.835
      C     3.631    1.527    2.140
      C     3.949    1.463    3.499
      C     3.668    2.546    4.335
```

C	3.079	3.694	3.799
C	2.749	3.744	2.442
C	-0.370	1.867	0.839
C	-0.574	2.945	1.705
C	-0.183	2.853	3.044
C	0.407	1.679	3.519
C	0.616	0.604	2.651
C	-0.206	-3.386	0.509
C	-0.987	-4.427	1.021
C	-2.024	-4.145	1.914
C	-2.284	-2.821	2.278
C	-1.506	-1.783	1.758
H	-2.626	-4.951	2.321
H	-0.787	-5.452	0.725
H	0.590	-3.609	-0.189
H	-1.745	-0.762	2.032
H	-3.094	-2.599	2.967
H	2.876	4.547	4.439
H	3.908	2.498	5.392
H	4.415	0.571	3.907
H	3.892	0.691	1.510
H	2.293	4.648	2.057
H	-1.036	3.856	1.337
H	-0.684	1.951	-0.195
H	1.074	-0.308	3.019
H	0.706	1.603	4.560
H	-0.337	3.693	3.714
H	0.482	4.907	-2.511
H	1.550	4.142	-3.720
H	0.015	3.337	-3.213
H	3.067	1.558	-4.178
H	2.001	0.264	-4.789
H	1.377	1.912	-4.618
H	1.242	-2.085	-4.959
H	1.215	-3.375	-2.589
H	-1.372	-3.927	-1.961
H	-2.934	-2.922	-3.925
H	-1.323	-1.769	-5.774
H	-0.869	1.042	-4.349
H	-2.343	-0.945	-0.784
H	-3.101	0.119	-3.147
XX	-0.930	0.022	-2.300
XX	-0.633	-2.805	-3.832

Complex 11a E=-293.79779 a.u.

Pd	1.050	-0.049	-1.937
P	1.189	-1.822	-3.494
N	-2.069	-2.630	-0.946
N	-1.086	-2.247	-0.096
C	2.186	-0.026	-0.026
C	2.656	-1.192	-0.603
C	-2.180	-1.920	-2.237
C	-1.626	-2.807	-3.310
C	-0.255	-2.872	-3.824
C	-1.092	-3.160	0.883
C	-2.065	-4.158	0.654
C	-2.675	-3.786	-0.532
C	3.924	-1.315	-1.361
C	4.360	-0.312	-2.246
C	5.508	-0.482	-3.017
C	6.280	-1.641	-2.880
C	5.894	-2.619	-1.961
C	4.716	-2.469	-1.223
Si	-0.187	1.517	-3.089
H	-3.488	-4.249	-1.074
H	-2.324	-5.007	1.272
H	-1.547	-1.033	-2.118
H	0.494	1.302	-1.273
C	2.368	-3.229	-3.184
C	1.854	-1.219	-5.140
C	-0.160	-4.115	-4.541
C	-2.296	-3.989	-3.759
C	-0.097	-2.989	1.991
C	-3.613	-1.453	-2.458
H	2.205	-2.130	-0.279
H	2.762	0.899	-0.077
H	1.414	-0.077	0.737
H	3.767	0.597	-2.343
H	5.791	0.284	-3.738
H	7.167	-1.784	-3.496
H	6.498	-3.518	-1.840
H	4.407	-3.252	-0.531
Cl	0.582	3.478	-3.027
Cl	-0.303	1.215	-5.196
Cl	-2.232	1.722	-2.591
Fe	-1.653	-2.987	-5.344
C	-1.277	-1.613	-6.820
C	3.578	-3.369	-3.873
C	-3.372	-2.412	-6.225

C	3.004	-2.283	4.932
C	0.672	-5.411	1.674
C	1.728	-3.816	3.341
C	-2.482	-1.293	-6.112
C	0.761	-4.036	2.353
C	4.376	-4.498	-3.662
C	1.882	-2.552	3.920
C	0.999	-1.526	3.571
C	-0.031	-1.756	2.652
C	2.017	-4.171	-2.211
C	4.009	-5.449	-2.706
C	-1.408	-4.817	-4.519
C	2.836	-5.277	-1.968
C	-1.088	-0.670	2.393
C	-2.713	-3.425	-6.997
C	-1.415	-2.935	-7.357
C	1.846	-1.980	-6.314
C	2.396	-1.477	-7.497
C	2.431	0.054	-5.176
C	2.974	-0.206	-7.518
C	2.993	0.561	-6.351
H	-0.131	-5.994	2.146
H	1.416	-2.968	-6.333
H	3.436	-1.285	4.764
H	2.368	-4.631	3.660
H	2.585	-2.327	5.948
H	-0.460	-0.930	-7.017
H	5.287	-4.632	-4.238
H	-4.368	-2.479	-5.801
H	0.464	-5.306	0.599
H	1.616	-5.968	1.775
H	0.759	-4.575	-4.888
H	3.811	-3.027	4.844
H	-2.708	-0.346	-5.635
H	1.114	-0.546	4.023
H	-3.690	-0.889	-3.399
H	-2.090	-1.124	2.386
H	4.636	-6.319	-2.536
H	1.101	-4.045	-1.643
H	-3.923	-0.798	-1.629
H	-1.622	-5.791	-4.945
H	-1.073	0.100	3.178
H	-3.326	-4.253	-3.545
H	2.559	-6.001	-1.208
H	-4.312	-2.300	-2.502

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H    -0.913   -0.181    1.424
H     3.915   -2.613   -4.571
H    -3.123   -4.396   -7.257
H    -0.681   -3.458   -7.961
H     2.374   -2.076   -8.403
H     2.440    0.665   -4.283
H     3.405    0.184   -8.435
H     3.443    1.548   -6.356
XX   -1.147   -3.713   -3.989
XX   -2.250   -2.336   -6.700

Complex 11b E=-293.79524 a.u.
Pd    0.501    0.289   -2.253
P     0.646   -1.435   -3.826
N    -2.634   -2.131   -1.363
N    -1.591   -1.808   -0.560
C     1.844    0.423   -0.395
C     2.724   -0.141   -1.292
C    -2.734   -1.443   -2.666
C    -2.198   -2.351   -3.731
C    -0.827   -2.416   -4.245
C    -1.624   -2.706    0.434
C    -2.679   -3.627    0.264
C    -3.307   -3.228   -0.903
C     3.227   -1.522   -1.290
C     4.320   -1.834   -2.120
C     4.908   -3.098   -2.082
C     4.416   -4.073   -1.213
C     3.327   -3.779   -0.382
C     2.731   -2.522   -0.432
Si   -0.745    1.908   -3.290
H    -4.181   -3.628   -1.404
H    -2.981   -4.438    0.915
H    -2.076   -0.570   -2.563
H    -0.123    1.594   -1.543
C     1.715   -2.948   -3.627
C     1.328   -0.707   -5.400
C    -0.752   -3.645   -4.998
C    -2.877   -3.526   -4.176
C    -0.576   -2.609    1.507
C    -4.154   -0.945   -2.890
H     3.290    0.542   -1.931
H     1.844    1.495   -0.223
H     1.384   -0.184    0.379
H     4.721   -1.068   -2.787
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H	5.759	-3.313	-2.727
H	4.889	-5.053	-1.176
H	2.953	-4.532	0.311
H	1.864	-2.307	0.191
Cl	0.246	3.767	-3.391
Cl	-1.047	1.523	-5.363
Cl	-2.711	2.356	-2.658
Fe	-2.244	-2.521	-5.771
C	-1.894	-1.131	-7.238
C	2.878	-3.154	-4.377
C	-3.968	-2.008	-6.684
C	2.654	-2.214	4.369
C	-0.077	-5.110	1.243
C	1.177	-3.598	2.844
C	-3.126	-0.856	-6.558
C	0.170	-3.735	1.882
C	3.513	-4.399	-4.345
C	1.484	-2.347	3.386
C	0.716	-1.236	3.022
C	-0.346	-1.371	2.121
C	1.307	-3.917	-2.706
C	3.035	-5.408	-3.504
C	-1.999	-4.349	-4.953
C	1.949	-5.158	-2.662
C	-1.258	-0.168	1.827
C	-3.258	-2.996	-7.443
C	-1.972	-2.457	-7.778
C	1.271	-1.345	-6.643
C	1.792	-0.725	-7.782
C	1.960	0.536	-5.303
C	2.392	0.533	-7.683
C	2.480	1.163	-6.439
H	-0.928	-5.593	1.744
H	0.824	-2.323	-6.742
H	2.939	-1.163	4.526
H	1.735	-4.469	3.174
H	2.361	-2.652	5.334
H	-1.096	-0.420	-7.416
H	4.380	-4.581	-4.972
H	-4.972	-2.111	-6.283
H	-0.289	-5.011	0.169
H	0.802	-5.764	1.347
H	0.147	-4.078	-5.422
H	3.530	-2.755	3.979
H	-3.407	0.089	-6.108

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H     0.945   -0.264    3.445
H    -4.208   -0.357   -3.817
H    -2.311   -0.488    1.817
H     3.513   -6.383   -3.500
H     0.481   -3.711   -2.034
H    -4.458   -0.302   -2.049
H    -2.225   -5.315   -5.395
H    -1.153    0.612    2.596
H    -3.900   -3.794   -3.935
H     1.604   -5.924   -1.974
H    -4.869   -1.776   -2.963
H    -1.008    0.272    0.851
H     3.291   -2.361   -4.990
H    -3.626   -3.981   -7.712
H    -1.207   -2.953   -8.367
H     1.731   -1.221   -8.746
H     2.048    1.022   -4.337
H     2.789    1.019   -8.569
H     2.952    2.136   -6.354
XX   -1.728   -3.251   -4.421
XX   -2.841   -1.890   -7.137


Complex 11c E=-293.78392 a.u.

Pd    0.447    1.007   -1.308
P     0.579   -0.913   -2.627
N    -2.709   -1.545   -0.497
N    -1.756   -1.156    0.381
Si    1.995    0.427    0.306
Cl    3.889    0.669   -0.579
Cl    2.178    1.355    2.190
Cl    1.953   -1.600    0.908
C    -2.769   -0.824   -1.779
C    -2.232   -1.697   -2.872
C    -0.861   -1.762   -3.386
C    -1.788   -2.058    1.368
C    -2.760   -3.053    1.113
C    -3.332   -2.692   -0.094
C    -0.918    2.280   -2.824
C    -0.570    2.997   -1.692
C    -0.319    2.534   -4.159
C     0.003    3.844   -4.552
C     0.625    4.094   -5.777
C     0.977    3.035   -6.617
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C	0.621	1.733	-6.258
C	-0.058	1.494	-5.065
H	-4.131	-3.154	-0.660
H	-3.044	-3.900	1.726
H	-2.090	0.025	-1.627
H	-1.239	3.069	-0.837
H	-1.849	1.705	-2.818
H	0.928	1.928	-0.077
C	1.401	-2.427	-1.927
C	1.887	-0.474	-3.903
C	-0.801	-2.945	-4.199
C	-2.917	-2.859	-3.347
C	-0.823	-1.888	2.519
C	-4.171	-0.287	-2.026
H	0.225	3.743	-1.738
H	-0.263	4.674	-3.898
H	0.845	5.118	-6.074
H	1.517	3.216	-7.545
H	0.900	0.903	-6.904
H	-0.358	0.480	-4.798
Fe	-2.337	-1.850	-4.916
C	-2.849	-0.119	-5.872
C	2.796	-2.540	-1.899
C	-3.796	-2.198	-6.275
C	1.956	-1.322	5.810
C	-0.304	-4.406	2.482
C	0.708	-2.816	4.153
C	-4.005	-0.933	-5.636
C	-0.150	-2.993	3.062
C	3.403	-3.701	-1.415
C	0.967	-1.539	4.659
C	0.309	-0.441	4.099
C	-0.597	-0.607	3.045
C	0.623	-3.456	-1.382
C	2.618	-4.755	-0.940
C	-2.040	-3.665	-4.145
C	1.226	-4.633	-0.931
C	-1.338	0.625	2.500
C	-2.509	-2.170	-6.906
C	-1.925	-0.885	-6.661
C	2.374	-1.364	-4.866
C	3.247	-0.920	-5.864
C	2.412	0.822	-3.860
C	3.709	0.399	-5.856
C	3.308	1.265	-4.837

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H    -1.138   -4.916    2.985
H     2.096   -2.406   -4.844
H     2.668   -0.527    5.538
H     1.181   -3.678    4.611
H     1.400   -1.014    6.708
H    -2.732    0.914   -5.564
H     4.486   -3.785   -1.407
H    -4.490   -3.032   -6.281
H    -0.489   -4.374    1.401
H     0.613   -4.995    2.637
H     0.078   -3.343   -4.682
H     2.526   -2.235    6.041
H    -4.904   -0.632   -5.109
H     0.506    0.548    4.499
H    -4.179    0.339   -2.931
H    -2.405    0.397    2.360
H     3.088   -5.665   -0.579
H    -0.453   -3.349   -1.305
H    -4.486    0.332   -1.172
H    -2.273   -4.610   -4.626
H    -1.270    1.480    3.189
H    -3.946   -3.122   -3.128
H     0.615   -5.455   -0.572
H    -4.899   -1.101   -2.148
H    -0.899    0.925    1.537
H     3.423   -1.728   -2.248
H    -2.060   -2.978   -7.474
H    -0.980   -0.545   -7.062
H     3.570   -1.602   -6.644
H     2.119    1.498   -3.064
H     4.378    0.747   -6.636
H     3.689    2.281   -4.804
XX   -1.771   -2.582   -3.588
XX   -3.012   -1.260   -6.266

Complex 12a E=-293.79636 a.u.

Pd    0.261    0.505   -2.560
P     0.307   -1.138   -4.115
N    -2.939   -1.888   -1.586
N    -1.911   -1.530   -0.780
C     1.420    0.935   -0.580
C     1.747   -0.347   -1.251
C    -3.052   -1.208   -2.893
C    -2.495   -2.126   -3.937
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C	-1.124	-2.191	-4.451
C	-1.899	-2.441	0.202
C	-2.906	-3.413	0.017
C	-3.554	-3.027	-1.143
C	3.033	-0.521	-1.939
C	3.566	0.476	-2.783
C	4.741	0.258	-3.497
C	5.441	-0.947	-3.357
C	4.954	-1.925	-2.485
C	3.755	-1.720	-1.798
Si	-1.052	2.132	-3.667
H	-4.400	-3.469	-1.654
H	-3.161	-4.255	0.649
H	-2.416	-0.319	-2.798
H	0.725	1.678	-1.225
C	1.532	-2.505	-3.825
C	0.933	-0.467	-5.740
C	-1.018	-3.439	-5.154
C	-3.157	-3.320	-4.366
C	-0.847	-2.290	1.264
C	-4.481	-0.745	-3.122
H	1.361	-1.249	-0.773
H	2.288	1.583	-0.425
H	0.860	0.817	0.347
H	3.035	1.420	-2.903
H	5.109	1.029	-4.176
H	6.354	-1.120	-3.926
H	5.504	-2.858	-2.354
H	3.379	-2.493	-1.127
Cl	-0.111	4.041	-3.564
Cl	-1.410	1.934	-5.761
Cl	-3.015	2.513	-2.924
Fe	-2.521	-2.339	-5.972
C	-2.182	-0.948	-7.443
C	2.732	-2.614	-4.537
C	-4.245	-1.862	-6.904
C	2.395	-1.659	4.068
C	-0.191	-4.749	0.973
C	0.993	-3.167	2.561
C	-3.424	-0.693	-6.774
C	-0.020	-3.365	1.616
C	3.555	-3.729	-4.349
C	1.225	-1.899	3.106
C	0.375	-0.843	2.766
C	-0.696	-1.045	1.889

C	1.223	-3.451	-2.843
C	3.222	-4.695	-3.395
C	-2.261	-4.152	-5.114
C	2.063	-4.547	-2.628
C	-1.706	0.087	1.634
C	-3.509	-2.839	-7.652
C	-2.231	-2.277	-7.979
C	0.932	-1.204	-6.929
C	1.406	-0.640	-8.117
C	1.466	0.826	-5.750
C	1.906	0.664	-8.123
C	1.941	1.396	-6.934
H	-0.993	-5.291	1.494
H	0.569	-2.219	-6.948
H	2.871	-0.691	3.851
H	1.609	-4.003	2.874
H	2.011	-1.647	5.099
H	-1.402	-0.218	-7.621
H	4.457	-3.841	-4.942
H	-5.249	-1.982	-6.511
H	-0.444	-4.660	-0.094
H	0.735	-5.339	1.044
H	-0.099	-3.881	-5.523
H	3.158	-2.446	3.979
H	-3.723	0.248	-6.327
H	0.549	0.139	3.193
H	-4.552	-0.176	-4.060
H	-2.730	-0.313	1.683
H	3.865	-5.557	-3.248
H	0.324	-3.335	-2.246
H	-4.797	-0.092	-2.293
H	-2.469	-5.132	-5.530
H	-1.618	0.881	2.391
H	-4.182	-3.590	-4.140
H	1.815	-5.281	-1.868
H	-5.178	-1.592	-3.175
H	-1.546	0.534	0.643
H	3.040	-1.844	-5.234
H	-3.857	-3.831	-7.921
H	-1.454	-2.758	-8.565
H	1.385	-1.216	-9.037
H	1.513	1.396	-4.831
H	2.267	1.106	-9.046
H	2.337	2.407	-6.929
XX	-2.010	-3.038	-4.605

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XX   -3.116   -1.725   -7.347

Complex 12b E=-293.78950 a.u.

Pd    0.653    0.149   -2.336
P     0.659   -1.419   -3.946
N    -2.647   -2.130   -1.368
N    -1.598   -1.826   -0.565
C     1.863    0.555   -0.371
C     2.570   -0.220   -1.419
C    -2.738   -1.440   -2.670
C    -2.198   -2.351   -3.731
C    -0.827   -2.416   -4.245
C    -1.638   -2.735    0.420
C    -2.703   -3.643    0.243
C    -3.330   -3.226   -0.918
C     3.181   -1.541   -1.258
C     4.292   -1.846   -2.074
C     4.930   -3.080   -1.999
C     4.461   -4.054   -1.113
C     3.359   -3.770   -0.297
C     2.732   -2.527   -0.359
Si   -0.823    1.724   -3.305
H    -4.202   -3.614   -1.430
H    -3.012   -4.459    0.884
H    -2.076   -0.571   -2.564
H     0.897    1.114   -0.787
C     1.835   -2.855   -3.802
C     1.227   -0.667   -5.552
C    -0.748   -3.641   -5.002
C    -2.868   -3.538   -4.166
C    -0.585   -2.661    1.492
C    -4.154   -0.936   -2.899
H     3.160    0.412   -2.093
H     2.409    1.453   -0.051
H     1.520   -0.027    0.487
H     4.652   -1.087   -2.772
H     5.787   -3.290   -2.637
H     4.939   -5.032   -1.067
H     2.978   -4.528    0.386
H     1.870   -2.320    0.270
Cl    0.319    3.529   -3.129
Cl   -1.139    1.602   -5.412
Cl   -2.753    2.302   -2.603
Fe   -2.259   -2.529   -5.766
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C	-1.960	-1.125	-7.239
C	3.005	-2.947	-4.562
C	-4.005	-2.055	-6.662
C	2.635	-2.349	4.375
C	-0.111	-5.162	1.190
C	1.144	-3.692	2.828
C	-3.190	-0.881	-6.545
C	0.144	-3.802	1.855
C	3.751	-4.129	-4.551
C	1.471	-2.451	3.382
C	0.728	-1.323	3.019
C	-0.333	-1.431	2.114
C	1.516	-3.875	-2.900
C	3.370	-5.191	-3.726
C	-1.989	-4.356	-4.947
C	2.265	-5.054	-2.880
C	-1.220	-0.209	1.825
C	-3.278	-3.024	-7.429
C	-2.011	-2.452	-7.779
C	1.166	-1.334	-6.780
C	1.587	-0.699	-7.952
C	1.780	0.617	-5.502
C	2.094	0.602	-7.901
C	2.196	1.259	-6.672
H	-0.970	-5.648	1.676
H	0.796	-2.345	-6.839
H	2.924	-1.304	4.563
H	1.681	-4.576	3.157
H	2.336	-2.813	5.326
H	-1.193	-0.386	-7.438
H	4.629	-4.222	-5.182
H	-5.002	-2.181	-6.252
H	-0.314	-5.040	0.116
H	0.762	-5.824	1.288
H	0.149	-4.060	-5.443
H	3.510	-2.884	3.974
H	-3.493	0.062	-6.104
H	0.976	-0.357	3.447
H	-4.199	-0.328	-3.813
H	-2.280	-0.507	1.824
H	3.935	-6.118	-3.736
H	0.678	-3.756	-2.221
H	-4.467	-0.311	-2.048
H	-2.210	-5.322	-5.389
H	-1.092	0.572	2.588

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H    -3.889   -3.811   -3.924
H     1.990   -5.861   -2.208
H    -4.868   -1.766   -2.998
H    -0.970    0.219    0.844
H     3.343   -2.112   -5.165
H    -3.627   -4.016   -7.697
H    -1.245   -2.925   -8.386
H     1.520   -1.218   -8.903
H     1.888    1.121   -4.548
H     2.408    1.100   -8.813
H     2.599    2.266   -6.625
XX   -1.725   -3.252   -4.419
XX   -2.886   -1.909   -7.126
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Complex 12c E=-293.75970 a.u.

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Pd    0.374    0.995   -1.453
P     0.578   -0.891   -2.649
N    -2.714   -1.540   -0.495
N    -1.758   -1.153    0.384
Si    1.957    0.344    0.235
Cl    3.910    0.637   -0.578
Cl    2.057    1.476    2.041
Cl    2.017   -1.649    0.999
C    -2.772   -0.823   -1.779
C    -2.232   -1.697   -2.872
C    -0.861   -1.762   -3.386
C    -1.797   -2.053    1.373
C    -2.773   -3.045    1.119
C    -3.341   -2.686   -0.091
C    -0.839    2.147   -2.810
C    -0.706    3.192   -1.727
C    -0.279    2.479   -4.148
C     0.043    3.799   -4.519
C     0.642    4.081   -5.748
C     0.971    3.049   -6.628
C     0.606    1.737   -6.305
C    -0.047    1.471   -5.105
H    -4.138   -3.149   -0.660
H    -3.068   -3.887    1.732
H    -2.091    0.025   -1.632
H    -1.100    2.841   -0.755
H    -1.823    1.673   -2.872
H    -1.259    4.125   -1.918
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C	1.393	-2.374	-1.881
C	1.892	-0.457	-3.912
C	-0.794	-2.948	-4.191
C	-2.913	-2.862	-3.348
C	-0.831	-1.875	2.523
C	-4.171	-0.288	-2.031
H	0.344	3.520	-1.617
H	-0.188	4.625	-3.850
H	0.859	5.114	-6.020
H	1.492	3.257	-7.564
H	0.868	0.920	-6.979
H	-0.336	0.450	-4.857
Fe	-2.332	-1.861	-4.919
C	-2.834	-0.139	-5.897
C	2.788	-2.487	-1.846
C	-3.797	-2.216	-6.270
C	1.991	-1.271	5.772
C	-0.379	-4.408	2.577
C	0.688	-2.786	4.179
C	-3.996	-0.941	-5.647
C	-0.184	-2.978	3.101
C	3.393	-3.628	-1.314
C	0.982	-1.501	4.640
C	0.340	-0.407	4.055
C	-0.580	-0.585	3.016
C	0.613	-3.383	-1.304
C	2.606	-4.666	-0.810
C	-2.032	-3.671	-4.138
C	1.214	-4.547	-0.817
C	-1.309	0.647	2.452
C	-2.512	-2.206	-6.904
C	-1.918	-0.922	-6.678
C	2.378	-1.354	-4.869
C	3.246	-0.916	-5.874
C	2.426	0.835	-3.871
C	3.707	0.403	-5.876
C	3.315	1.274	-4.856
H	-1.226	-4.873	3.100
H	2.102	-2.396	-4.837
H	2.699	-0.480	5.482
H	1.144	-3.644	4.662
H	1.450	-0.956	6.676
H	-2.710	0.898	-5.604
H	4.476	-3.709	-1.293
H	-4.498	-3.045	-6.263

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H    -0.565   -4.412    1.495
H     0.520   -5.018    2.753
H     0.088   -3.345   -4.670
H     2.565   -2.182    6.001
H    -4.891   -0.626   -5.122
H     0.562    0.589    4.423
H    -4.177    0.336   -2.937
H    -2.379    0.430    2.320
H     3.074   -5.562   -0.413
H    -0.464   -3.273   -1.233
H    -4.488    0.334   -1.179
H    -2.260   -4.618   -4.615
H    -1.229    1.511    3.129
H    -3.942   -3.127   -3.130
H     0.603   -5.363   -0.445
H    -4.898   -1.102   -2.153
H    -0.871    0.930    1.484
H     3.416   -1.691   -2.229
H    -2.070   -3.024   -7.463
H    -0.970   -0.595   -7.084
H     3.566   -1.602   -6.651
H     2.149    1.511   -3.071
H     4.368    0.749   -6.664
H     3.697    2.289   -4.831
XX   -1.767   -2.584   -3.586
XX   -3.006   -1.284   -6.274

Complex 13a E=-293.81420 a.u.

Pd    0.845    0.344   -2.352
P     0.369   -1.249   -3.992
N    -2.862   -1.897   -1.559
N    -1.798   -1.573   -0.785
C     2.576    2.773   -1.043
C     1.935    1.416   -0.868
C    -3.004   -1.214   -2.861
C    -2.495   -2.126   -3.937
C    -1.124   -2.191   -4.451
C    -1.804   -2.471    0.209
C    -2.859   -3.399    0.063
C    -3.518   -3.000   -1.087
C     2.734    0.202   -1.041
C     4.022    0.172   -1.651
C     4.693   -1.025   -1.832
C     4.116   -2.247   -1.433
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C	2.846	-2.256	-0.874
C	2.148	-1.050	-0.692
Si	-0.399	2.089	-3.129
H	-4.393	-3.410	-1.576
H	-3.138	-4.216	0.716
H	-2.358	-0.332	-2.787
H	3.048	2.900	-2.025
C	1.490	-2.706	-3.725
C	1.105	-0.546	-5.558
C	-1.055	-3.396	-5.237
C	-3.191	-3.266	-4.441
C	-0.738	-2.355	1.264
C	-4.436	-0.733	-3.038
H	1.259	1.368	-0.007
H	3.349	2.932	-0.272
H	1.835	3.572	-0.938
H	4.491	1.108	-1.951
H	5.688	-1.022	-2.276
H	4.674	-3.175	-1.551
H	2.393	-3.190	-0.543
H	1.194	-1.057	-0.169
Cl	0.483	3.981	-3.475
Cl	-1.293	1.714	-5.030
Cl	-2.066	2.523	-1.895
Fe	-2.518	-2.191	-5.980
C	-2.121	-0.701	-7.331
C	2.785	-2.749	-4.254
C	-4.216	-1.594	-6.892
C	2.450	-1.893	4.167
C	-0.211	-4.849	1.002
C	1.011	-3.331	2.619
C	-3.366	-0.462	-6.663
C	0.015	-3.474	1.646
C	3.578	-3.886	-4.072
C	1.310	-2.076	3.158
C	0.554	-0.967	2.767
C	-0.495	-1.105	1.851
C	1.029	-3.769	-2.942
C	3.097	-4.964	-3.325
C	-2.321	-4.068	-5.249
C	1.824	-4.902	-2.750
C	-1.369	0.112	1.506
C	-3.497	-2.530	-7.706
C	-2.200	-1.980	-7.974
C	0.998	-1.150	-6.815

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C     1.540   -0.536   -7.948
C     1.837    0.640   -5.442
C     2.219    0.679   -7.830
C     2.374    1.264   -6.572
H    -1.032   -5.362    1.524
H     0.497   -2.096   -6.933
H     3.105   -1.073    3.836
H     1.561   -4.203    2.958
H     2.023   -1.639    5.148
H    -1.310    0.012   -7.425
H     4.570   -3.929   -4.509
H    -5.230   -1.715   -6.524
H    -0.459   -4.751   -0.065
H     0.693   -5.473    1.073
H    -0.147   -3.847   -5.620
H     3.059   -2.804    4.269
H    -3.649    0.454   -6.157
H     0.788    0.007    3.183
H    -4.534   -0.155   -3.968
H    -2.430   -0.177    1.481
H     3.711   -5.849   -3.189
H     0.049   -3.716   -2.479
H    -4.716   -0.083   -2.194
H    -2.556   -5.015   -5.724
H    -1.256    0.914    2.251
H    -4.218   -3.527   -4.212
H     1.455   -5.730   -2.154
H    -5.145   -1.571   -3.075
H    -1.079    0.509    0.523
H     3.186   -1.906   -4.804
H    -3.869   -3.487   -8.057
H    -1.433   -2.434   -8.593
H     1.432   -1.004   -8.922
H     1.998    1.084   -4.467
H     2.627    1.164   -8.712
H     2.913    2.201   -6.470
XX   -2.035   -3.002   -4.664
XX   -3.078   -1.455   -7.310

Complex 13b E=-293.81070 a.u.

Pd    0.897    0.430   -2.390
P     0.349   -1.195   -4.019
N    -2.857   -1.872   -1.566
N    -1.749   -1.581   -0.843
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C	2.770	2.810	-1.323
C	2.086	1.493	-1.009
C	-3.016	-1.208	-2.875
C	-2.495	-2.126	-3.937
C	-1.124	-2.191	-4.451
C	-1.750	-2.462	0.165
C	-2.848	-3.348	0.075
C	-3.537	-2.942	-1.054
C	2.865	0.247	-1.155
C	3.692	0.025	-2.292
C	4.407	-1.162	-2.440
C	4.321	-2.166	-1.472
C	3.501	-1.979	-0.351
C	2.774	-0.802	-0.204
Si	-0.567	2.092	-2.867
H	-4.445	-3.327	-1.504
H	-3.134	-4.141	0.756
H	-2.380	-0.317	-2.818
H	3.330	2.793	-2.268
C	1.525	-2.603	-3.714
C	0.997	-0.504	-5.631
C	-1.041	-3.413	-5.204
C	-3.189	-3.266	-4.442
C	-0.670	-2.382	1.213
C	-4.456	-0.746	-3.054
H	1.536	1.536	-0.063
H	3.491	3.043	-0.520
H	2.055	3.637	-1.379
H	3.802	0.816	-3.032
H	5.044	-1.298	-3.314
H	4.894	-3.085	-1.586
H	3.441	-2.753	0.414
H	2.158	-0.645	0.677
Cl	0.139	4.051	-3.236
Cl	-1.613	1.709	-4.694
Cl	-2.117	2.387	-1.462
Fe	-2.479	-2.207	-5.986
C	-2.064	-0.665	-7.262
C	2.725	-2.763	-4.415
C	-4.135	-1.681	-7.015
C	2.312	-2.114	4.354
C	-0.268	-4.907	0.985
C	0.936	-3.459	2.669
C	-3.371	-0.511	-6.695
C	-0.005	-3.541	1.637

C	3.546	-3.864	-4.154
C	1.264	-2.225	3.239
C	0.625	-1.070	2.781
C	-0.337	-1.138	1.767
C	1.185	-3.515	-2.710
C	3.191	-4.786	-3.165
C	-2.310	-4.080	-5.230
C	2.016	-4.604	-2.432
C	-1.023	0.150	1.285
C	-3.302	-2.554	-7.790
C	-2.021	-1.927	-7.942
C	1.048	-1.230	-6.826
C	1.464	-0.620	-8.013
C	1.470	0.812	-5.626
C	1.873	0.716	-8.009
C	1.886	1.430	-6.808
H	-1.083	-5.413	1.524
H	0.774	-2.272	-6.852
H	3.165	-1.525	3.985
H	1.418	-4.361	3.029
H	1.870	-1.602	5.222
H	-1.283	0.088	-7.257
H	4.463	-4.002	-4.718
H	-5.166	-1.866	-6.734
H	-0.540	-4.804	-0.075
H	0.630	-5.541	1.033
H	-0.126	-3.883	-5.543
H	2.677	-3.100	4.678
H	-3.744	0.377	-6.198
H	0.887	-0.113	3.222
H	-4.560	-0.174	-3.986
H	-2.114	0.013	1.262
H	3.830	-5.640	-2.964
H	0.271	-3.375	-2.143
H	-4.742	-0.095	-2.213
H	-2.539	-5.036	-5.690
H	-0.805	1.005	1.941
H	-4.217	-3.529	-4.216
H	1.747	-5.306	-1.649
H	-5.157	-1.591	-3.088
H	-0.666	0.393	0.274
H	3.035	-2.040	-5.160
H	-3.591	-3.520	-8.193
H	-1.185	-2.321	-8.510
H	1.471	-1.185	-8.940

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H     1.520    1.365   -4.696
H     2.180    1.196   -8.933
H     2.220    2.462   -6.794
XX   -2.030   -3.008   -4.653
XX   -2.977   -1.469   -7.338

Complex 13c E=-293.81580 a.u.

Pd    1.078   -0.036   -1.893
P     0.650   -1.541   -3.639
N    -2.624   -2.214   -1.348
N    -1.691   -1.834   -0.447
C     1.819    1.552    0.769
C     2.339    0.984   -0.536
C    -2.706   -1.478   -2.624
C    -2.198   -2.351   -3.731
C    -0.827   -2.416   -4.245
C    -1.761   -2.744    0.534
C    -2.732   -3.731    0.253
C    -3.267   -3.358   -0.968
C     2.927   -0.364   -0.594
C     3.936   -0.685   -1.549
C     4.450   -1.974   -1.647
C     3.962   -2.997   -0.821
C     2.937   -2.725    0.086
C     2.419   -1.433    0.195
Si    0.092    1.896   -2.546
H    -4.047   -3.812   -1.567
H    -3.044   -4.572    0.860
H    -2.033   -0.621   -2.495
H     1.205    2.440    0.587
C     1.684   -3.059   -3.346
C     1.508   -0.791   -5.120
C    -0.779   -3.569   -5.102
C    -2.928   -3.414   -4.345
C    -0.837   -2.573    1.709
C    -4.123   -0.954   -2.810
H     2.907    1.723   -1.110
H     2.662    1.858    1.410
H     1.214    0.843    1.343
H     4.326    0.107   -2.188
H     5.235   -2.189   -2.370
H     4.383   -3.999   -0.884
H     2.543   -3.516    0.721
H     1.645   -1.224    0.927
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Cl	1.328	3.605	-2.769
Cl	-0.847	1.768	-4.453
Cl	-1.463	2.553	-1.274
Fe	-2.171	-2.239	-5.777
C	-1.645	-0.658	-6.968
C	2.906	-3.287	-3.988
C	-3.802	-1.464	-6.679
C	1.903	-1.968	5.016
C	-0.172	-5.044	1.544
C	0.754	-3.469	3.296
C	-2.899	-0.409	-6.321
C	-0.095	-3.657	2.199
C	3.600	-4.479	-3.764
C	0.922	-2.201	3.860
C	0.183	-1.126	3.358
C	-0.719	-1.309	2.304
C	1.202	-3.994	-2.424
C	3.094	-5.431	-2.875
C	-2.071	-4.182	-5.200
C	1.901	-5.181	-2.190
C	-1.575	-0.125	1.824
C	-3.107	-2.362	-7.554
C	-1.772	-1.867	-7.730
C	1.443	-1.313	-6.416
C	2.091	-0.674	-7.477
C	2.290	0.346	-4.895
C	2.833	0.487	-7.247
C	2.937	0.995	-5.950
H	-1.024	-5.596	1.966
H	0.891	-2.216	-6.622
H	2.557	-1.115	4.777
H	1.290	-4.315	3.712
H	1.333	-1.739	5.929
H	-0.790	0.008	-6.960
H	4.537	-4.665	-4.280
H	-4.833	-1.558	-6.355
H	-0.290	-4.962	0.454
H	0.746	-5.622	1.732
H	0.126	-4.035	-5.478
H	2.535	-2.849	5.203
H	-3.145	0.472	-5.739
H	0.314	-0.143	3.798
H	-4.200	-0.361	-3.731
H	-2.617	-0.445	1.680
H	3.628	-6.362	-2.712

```
H     0.278   -3.797   -1.890
H    -4.395   -0.312   -1.958
H    -2.331   -5.080   -5.751
H    -1.575    0.698    2.554
H    -3.972   -3.646   -4.167
H     1.519   -5.906   -1.479
H    -4.851   -1.776   -2.863
H    -1.180    0.259    0.872
H     3.327   -2.549   -4.660
H    -3.518   -3.261   -8.003
H    -1.008   -2.308   -8.362
H     2.017   -1.079   -8.481
H     2.403    0.734   -3.889
H     3.328    0.991   -8.072
H     3.520    1.891   -5.762
XX   -1.758   -3.178   -4.525
XX   -2.643   -1.354   -7.048

Complex 13d E=-293.81468 a.u.

Pd    0.960    0.023   -1.893
P     0.631   -1.550   -3.586
N    -2.822   -2.116   -1.364
N    -2.146   -1.576   -0.328
C     1.354    1.715    0.740
C     2.073    0.975   -0.370
C    -2.745   -1.440   -2.675
C    -2.198   -2.351   -3.731
C    -0.827   -2.416   -4.245
C    -2.427   -2.360    0.724
C    -3.286   -3.419    0.358
C    -3.523   -3.227   -0.994
C     2.413   -0.450   -0.231
C     3.634   -0.988   -0.735
C     3.900   -2.347   -0.664
C     2.952   -3.236   -0.126
C     1.718   -2.752    0.295
C     1.438   -1.379    0.240
Si    0.368    1.991   -2.880
H    -4.126   -3.797   -1.689
H    -3.721   -4.197    0.973
H    -2.048   -0.606   -2.515
H     1.007    2.697    0.397
C     1.599   -3.086   -3.169
C     1.639   -0.897   -5.014
```

C	-0.775	-3.559	-5.111
C	-2.927	-3.407	-4.363
C	-1.765	-1.992	2.028
C	-4.122	-0.862	-2.984
H	2.885	1.561	-0.813
H	2.044	1.880	1.585
H	0.485	1.172	1.128
H	4.368	-0.307	-1.169
H	4.849	-2.730	-1.038
H	3.180	-4.297	-0.046
H	0.956	-3.436	0.664
H	0.476	-1.016	0.601
Cl	1.829	3.522	-2.989
Cl	-0.239	1.816	-4.912
Cl	-1.296	2.930	-1.964
Fe	-2.161	-2.226	-5.786
C	-1.571	-0.735	-7.075
C	2.949	-3.229	-3.507
C	-3.767	-1.335	-6.630
C	0.471	-0.785	5.544
C	-1.302	-4.469	2.539
C	-0.542	-2.576	4.032
C	-2.755	-0.353	-6.365
C	-1.213	-2.971	2.868
C	3.617	-4.426	-3.232
C	-0.355	-1.223	4.328
C	-0.934	-0.258	3.499
C	-1.694	-0.638	2.387
C	0.953	-4.110	-2.469
C	2.948	-5.473	-2.592
C	-2.067	-4.172	-5.217
C	1.617	-5.309	-2.198
C	-2.450	0.441	1.593
C	-3.205	-2.325	-7.502
C	-1.845	-1.959	-7.771
C	1.528	-1.344	-6.334
C	2.310	-0.777	-7.345
C	2.593	0.082	-4.713
C	3.223	0.235	-7.042
C	3.368	0.663	-5.721
H	-2.275	-4.853	2.877
H	0.838	-2.129	-6.598
H	1.128	0.054	5.270
H	-0.156	-3.327	4.713
H	-0.214	-0.460	6.342

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H    -0.673   -0.135   -7.165
H     4.659   -4.543   -3.515
H    -4.785   -1.322   -6.254
H    -1.187   -4.648    1.460
H    -0.509   -5.036    3.049
H     0.132   -4.015   -5.492
H     1.098   -1.605    5.925
H    -2.884    0.568   -5.807
H    -0.794    0.793    3.728
H    -4.103   -0.271   -3.908
H    -3.448    0.074    1.309
H     3.461   -6.409   -2.397
H    -0.070   -3.977   -2.133
H    -4.438   -0.202   -2.160
H    -2.326   -5.062   -5.782
H    -2.590    1.352    2.193
H    -3.977   -3.629   -4.209
H     1.100   -6.111   -1.680
H    -4.873   -1.657   -3.090
H    -1.893    0.709    0.684
H     3.491   -2.420   -3.982
H    -3.718   -3.200   -7.888
H    -1.155   -2.495   -8.414
H     2.206   -1.123   -8.369
H     2.739    0.396   -3.685
H     3.820    0.686   -7.830
H     4.081    1.443   -5.476
XX   -1.758   -3.172   -4.535
XX   -2.627   -1.345   -7.064

Complex 13e E=-293.78823 a.u.

Pd    0.705    0.883   -1.490
P     0.590   -1.181   -2.410
N    -2.654   -1.580   -0.456
N    -1.869   -1.063    0.516
Si    2.083    0.589    0.357
Cl    4.128    1.113    0.281
Cl    1.060    2.499    0.738
Cl    1.951   -0.558    2.121
C    -2.730   -0.856   -1.736
C    -2.232   -1.697   -2.872
C    -0.861   -1.762   -3.386
C    -1.999   -1.892    1.561
C    -2.866   -2.965    1.249
```

C	-3.271	-2.730	-0.055
C	-0.458	1.982	-2.950
C	-1.235	3.052	-2.208
C	0.685	2.413	-3.788
C	1.136	3.743	-3.914
C	2.311	4.031	-4.617
C	3.094	3.010	-5.160
C	2.630	1.691	-5.103
C	1.422	1.428	-4.480
H	-3.933	-3.289	-0.705
H	-3.208	-3.777	1.877
H	-2.043	-0.007	-1.601
H	-1.963	2.615	-1.515
H	-1.104	1.259	-3.455
H	-1.795	3.706	-2.899
C	0.801	-2.656	-1.223
C	2.143	-1.439	-3.471
C	-0.839	-2.896	-4.281
C	-2.998	-2.674	-3.573
C	-1.235	-1.529	2.818
C	-4.138	-0.313	-1.930
H	-0.573	3.702	-1.619
H	0.546	4.555	-3.496
H	2.617	5.068	-4.752
H	4.040	3.238	-5.649
H	3.209	0.876	-5.537
H	0.975	0.444	-4.509
Fe	-2.174	-1.500	-4.943
C	-2.864	0.343	-5.508
C	-0.160	-3.671	-1.121
C	-3.081	-1.614	-6.734
C	1.200	-0.342	6.218
C	-0.772	-4.010	3.332
C	0.092	-2.124	4.758
C	-3.776	-0.699	-5.877
C	-0.648	-2.510	3.634
C	0.032	-4.781	-0.293
C	0.311	-0.774	5.045
C	-0.295	0.195	4.243
C	-1.112	-0.175	3.169
C	1.938	-2.767	-0.411
C	1.186	-4.885	0.485
C	-2.155	-3.443	-4.439
C	2.133	-3.861	0.437
C	-1.873	0.927	2.413

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C    -1.735   -1.145   -6.885
C    -1.604    0.070   -6.135
C     2.125   -1.855   -4.809
C     3.284   -2.332   -5.427
C     3.397   -1.173   -2.911
C     4.511   -2.248   -4.766
C     4.572   -1.627   -3.517
H    -1.708   -4.389    3.767
H     1.221   -1.790   -5.401
H     0.565    0.081    7.011
H     0.506   -2.880    5.417
H     1.771   -1.186    6.632
H    -3.111    1.230   -4.934
H    -0.719   -5.564   -0.252
H    -3.498   -2.510   -7.183
H    -0.766   -4.194    2.251
H     0.068   -4.576    3.762
H     0.039   -3.475   -4.539
H     1.912    0.426    5.879
H    -4.815   -0.775   -5.571
H    -0.127    1.244    4.464
H    -4.207    0.250   -2.871
H    -2.897    0.597    2.182
H     1.343   -5.749    1.124
H     2.699   -2.006   -0.421
H    -4.394    0.361   -1.097
H    -2.434   -4.324   -5.009
H    -1.952    1.846    3.013
H    -4.052   -2.877   -3.418
H     3.022   -3.917    1.057
H    -4.877   -1.127   -1.949
H    -1.348    1.172    1.479
H    -1.082   -3.632   -1.679
H    -0.959   -1.612   -7.483
H    -0.746    0.731   -6.148
H     3.233   -2.760   -6.424
H     3.470   -0.591   -2.003
H     5.410   -2.653   -5.222
H     5.528   -1.494   -3.021
XX   -1.813   -2.487   -3.711
XX   -2.610   -0.611   -6.224

Complex 13f    E=-293.79110 a.u.
 Pd    0.488    0.913   -1.497
P     0.532   -1.041   -2.535
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N	-2.734	-1.527	-0.478
N	-1.857	-1.076	0.442
Si	1.924	0.756	0.405
Cl	3.980	1.247	0.120
Cl	1.245	2.416	1.600
Cl	2.077	-0.947	1.703
C	-2.780	-0.825	-1.775
C	-2.232	-1.697	-2.872
C	-0.861	-1.762	-3.386
C	-1.910	-1.955	1.454
C	-2.832	-2.994	1.175
C	-3.340	-2.685	-0.076
C	-0.642	2.060	-2.988
C	-1.077	3.248	-2.146
C	0.547	2.204	-3.831
C	1.796	2.524	-3.245
C	2.982	2.167	-3.904
C	2.924	1.678	-5.220
C	1.681	1.476	-5.855
C	0.508	1.714	-5.153
H	-4.081	-3.184	-0.684
H	-3.125	-3.826	1.806
H	-2.095	0.023	-1.636
H	-1.688	3.039	-1.247
H	-1.417	1.563	-3.604
H	-1.672	3.902	-2.846
C	1.029	-2.551	-1.496
C	1.932	-0.947	-3.748
C	-0.840	-2.961	-4.197
C	-2.981	-2.778	-3.420
C	-1.007	-1.680	2.641
C	-4.183	-0.304	-2.033
H	-0.204	3.849	-1.852
H	1.808	3.038	-2.276
H	3.937	2.213	-3.360
H	3.843	1.443	-5.758
H	1.622	1.056	-6.870
H	-0.473	1.499	-5.597
Fe	-2.299	-1.789	-4.953
C	-2.851	-0.054	-5.889
C	0.106	-3.568	-1.217
C	-3.644	-2.170	-6.413
C	1.773	-0.733	5.842
C	-0.494	-4.187	2.905
C	0.512	-2.410	4.382

C	-3.966	-0.944	-5.745
C	-0.340	-2.715	3.314
C	0.498	-4.751	-0.583
C	0.767	-1.082	4.739
C	0.088	-0.059	4.073
C	-0.840	-0.353	3.068
C	2.314	-2.681	-0.954
C	1.804	-4.892	-0.110
C	-2.116	-3.617	-4.198
C	2.707	-3.841	-0.280
C	-1.672	0.794	2.470
C	-2.326	-2.044	-6.962
C	-1.839	-0.734	-6.649
C	1.764	-1.281	-5.095
C	2.876	-1.506	-5.912
C	3.206	-0.571	-3.313
C	4.164	-1.309	-5.407
C	4.328	-0.809	-4.112
H	-1.377	-4.610	3.406
H	0.774	-1.363	-5.522
H	1.225	-0.373	6.725
H	0.986	-3.210	4.940
H	2.382	-1.603	6.131
H	-2.835	0.981	-5.570
H	-0.214	-5.560	-0.453
H	-4.285	-3.043	-6.487
H	-0.606	-4.281	1.818
H	0.389	-4.776	3.193
H	0.060	-3.429	-4.581
H	2.448	0.061	5.488
H	-4.905	-0.718	-5.251
H	0.286	0.972	4.347
H	-4.203	0.261	-2.977
H	-2.719	0.480	2.347
H	2.112	-5.806	0.387
H	3.032	-1.882	-1.035
H	-4.480	0.372	-1.216
H	-2.372	-4.553	-4.683
H	-1.668	1.678	3.125
H	-4.022	-3.004	-3.222
H	3.716	-3.927	0.112
H	-4.922	-1.116	-2.086
H	-1.264	1.089	1.492
H	-0.936	-3.466	-1.481
H	-1.800	-2.800	-7.536

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H    -0.917   -0.309   -7.028
H     2.739   -1.832   -6.938
H     3.329   -0.085   -2.354
H     5.031   -1.532   -6.020
H     5.322   -0.601   -3.730
XX   -1.803   -2.558   -3.617
XX   -2.920   -1.189   -6.325
```

Complex 14a E=-293.80337 a.u.

```
Pd    0.390   -0.832   -2.557
P     0.311   -1.731   -4.641
N    -2.374   -2.362   -2.211
N    -1.444   -1.684   -1.482
C     2.445    5.046   -1.687
C     1.226    4.107   -1.846
C    -2.826   -1.802   -3.497
C    -2.431   -2.648   -4.675
C    -1.122   -2.627   -5.335
C    -1.277   -2.411   -0.361
C    -2.071   -3.573   -0.386
C    -2.763   -3.504   -1.584
C     1.615    2.658   -2.060
C     2.366    2.264   -3.206
C     2.759    0.956   -3.378
C     2.415   -0.052   -2.422
C     1.720    0.345   -1.225
C     1.317    1.707   -1.094
Si    0.030    4.768   -3.143
H    -3.496   -4.171   -2.020
H    -2.171   -4.336    0.373
H    -2.293   -0.843   -3.567
H     3.046    4.716   -0.829
C     1.630   -3.025   -4.885
C     0.759   -0.584   -6.034
C    -1.186   -3.588   -6.395
C    -3.228   -3.615   -5.361
C    -0.364   -1.874    0.706
C    -4.317   -1.512   -3.397
H     0.623    4.162   -0.923
H     2.142    6.088   -1.516
H     3.085    5.017   -2.577
H     2.641    3.008   -3.954
H     3.359    0.684   -4.247
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H	2.994	-0.978	-2.426
H	1.798	-0.268	-0.327
H	0.809	2.022	-0.180
Cl	0.952	5.216	-4.953
Cl	-1.520	3.453	-3.527
Cl	-0.813	6.547	-2.459
Fe	-2.631	-2.210	-6.660
C	-2.444	-1.547	-8.562
C	2.928	-2.660	-5.259
C	-3.358	-0.320	-6.817
C	2.258	-0.231	3.744
C	0.792	-4.155	0.859
C	1.419	-2.176	2.312
C	-2.198	-0.473	-7.644
C	0.601	-2.697	1.303
C	3.903	-3.640	-5.467
C	1.329	-0.830	2.681
C	0.373	-0.015	2.067
C	-0.495	-0.535	1.100
C	1.338	-4.371	-4.642
C	3.592	-4.989	-5.272
C	-2.476	-4.217	-6.425
C	2.310	-5.353	-4.852
C	-1.588	0.364	0.498
C	-4.331	-1.288	-7.236
C	-3.765	-2.045	-8.315
C	1.183	-1.048	-7.283
C	1.520	-0.139	-8.289
C	0.639	0.790	-5.808
C	1.432	1.236	-8.050
C	0.989	1.701	-6.809
H	1.815	-4.502	1.072
H	1.255	-2.111	-7.480
H	1.660	0.058	4.622
H	2.132	-2.822	2.812
H	3.033	-0.943	4.064
H	-1.757	-1.905	-9.322
H	4.902	-3.353	-5.779
H	-3.490	0.428	-6.042
H	0.085	-4.794	1.405
H	0.626	-4.263	-0.223
H	-0.361	-3.860	-7.043
H	2.752	0.663	3.336
H	-1.332	0.175	-7.644
H	0.310	1.030	2.352

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      H    -4.683   -1.032   -4.315
      H    -2.549   -0.172    0.484
      H     4.345   -5.751   -5.446
      H     0.355   -4.659   -4.285
      H    -4.510   -0.835   -2.549
      H    -2.812   -4.989   -7.110
      H    -1.726    1.284    1.085
      H    -4.252   -3.873   -5.117
      H     2.069   -6.399   -4.687
      H    -4.891   -2.435   -3.232
      H    -1.318    0.648   -0.529
      H     3.186   -1.616   -5.389
      H    -5.323   -1.420   -6.818
      H    -4.250   -2.858   -8.846
      H     1.852   -0.500   -9.258
      H     0.272    1.150   -4.853
      H     1.706    1.942   -8.828
      H     0.914    2.767   -6.623
      XX   -2.086   -3.335   -5.635
      XX   -3.219   -1.135   -7.714


      Product 14b E=-100.09580 a.u.

C          2.8595      3.7693     -1.8059
C          1.8279      2.9538     -0.9966
C          2.1965      1.4926     -0.8126
C          2.5857      0.6938     -1.8993
C          2.9147     -0.6499     -1.7126
C          2.8572     -1.2210     -0.4378
C          2.4583     -0.4389      0.6472
C          2.1346      0.9056      0.4609
Si         0.0713      3.1234     -1.6658
H          2.9630      3.3955     -2.8302
H          1.7398      3.4076      0.0072
H          3.8456      3.6951     -1.3284
H          2.5784      4.8264     -1.8619
H          2.6244      1.1232     -2.9012
H          3.2195     -1.2568     -2.5650
H          3.1165     -2.2687     -0.2969
H          2.4018     -0.8765      1.6424
H          1.8266      1.5147      1.3110
Cl        -0.5077      5.1147     -1.6341
Cl        -0.1072      2.4485     -3.6166
Cl        -1.2529      2.0486     -0.4982
```

Complex 11a' -367.00044 a.u.

Pd	1.034	-0.094	-1.968
P	1.238	-1.861	-3.556
N	-2.076	-2.579	-0.945
N	-1.073	-2.205	-0.117
C	2.203	0.076	-0.036
C	2.725	-1.086	-0.567
C	-2.176	-1.896	-2.254
C	-1.626	-2.807	-3.310
C	-0.255	-2.872	-3.824
C	-1.068	-3.116	0.865
C	-2.057	-4.102	0.660
C	-2.687	-3.723	-0.514
C	4.019	-1.186	-1.275
C	4.476	-0.193	-2.160
C	5.671	-0.354	-2.857
C	6.453	-1.497	-2.662
C	6.033	-2.470	-1.753
C	4.823	-2.320	-1.074
C	2.373	-3.302	-3.224
C	1.854	-1.254	-5.202
C	3.528	-3.542	-3.977
C	4.306	-4.677	-3.731
C	2.015	-4.209	-2.211
C	3.942	-5.580	-2.732
C	2.795	-5.340	-1.969
C	1.845	-2.000	-6.393
C	2.394	-1.475	-7.563
C	2.440	0.019	-5.218
C	2.983	-0.208	-7.562
C	3.008	0.537	-6.384
Si	-0.256	1.552	-2.952
H	-3.519	-4.174	-1.041
H	-2.313	-4.948	1.286
H	-1.528	-1.015	-2.152
H	0.538	1.252	-1.266
C	-0.165	-4.119	-4.542
C	-2.298	-3.992	-3.746
C	-0.037	-2.945	1.943
C	-3.601	-1.417	-2.480
H	2.286	-2.034	-0.249
H	2.754	1.014	-0.092
H	1.418	0.027	0.713

H	3.861	0.691	-2.333
H	5.986	0.407	-3.571
H	7.376	-1.633	-3.225
H	6.635	-3.363	-1.591
H	4.485	-3.100	-0.392
H	1.416	-2.995	-6.439
H	5.204	-4.848	-4.324
H	4.550	-6.464	-2.546
H	1.113	-4.037	-1.623
H	2.501	-6.042	-1.188
H	3.829	-2.846	-4.756
H	2.363	-2.064	-8.479
H	2.440	0.615	-4.305
H	3.415	0.196	-8.477
H	3.454	1.531	-6.369
Cl	0.658	3.465	-2.996
Cl	-0.738	1.293	-4.999
Cl	-2.173	1.884	-2.117
Fe	-1.657	-3.005	-5.349
C	-1.312	-1.596	-6.791
C	-3.376	-2.530	-6.294
C	3.208	-2.213	4.716
C	0.687	-5.382	1.646
C	1.841	-3.763	3.223
C	-2.566	-1.358	-6.139
C	0.825	-3.994	2.288
C	2.030	-2.491	3.772
C	1.132	-1.467	3.455
C	0.059	-1.706	2.591
C	-1.411	-4.825	-4.502
C	-1.014	-0.626	2.375
C	-2.625	-3.491	-7.049
C	-1.349	-2.914	-7.354
H	-0.111	-5.937	2.160
H	3.608	-1.203	4.542
H	2.492	-4.576	3.524
H	2.856	-2.287	5.755
H	-0.520	-0.868	-6.924
H	-4.385	-2.662	-5.917
H	0.442	-5.299	0.577
H	1.622	-5.956	1.728
H	0.746	-4.564	-4.925
H	4.022	-2.937	4.561
H	-2.882	-0.425	-5.687
H	1.270	-0.482	3.890

```
      H    -3.667   -0.840   -3.413
      H    -2.014   -1.084    2.430
      H    -3.910   -0.767   -1.646
      H    -1.628   -5.799   -4.927
      H    -0.959    0.154    3.150
      H    -3.325   -4.254   -3.523
      H    -4.306   -2.258   -2.538
      H    -0.898   -0.148    1.393
      H    -2.965   -4.479   -7.340
      H    -0.570   -3.378   -7.951
      XX   -1.149   -3.715   -3.985
      XX   -2.243   -2.379   -6.722

Complex 11b' E= -366.99254 a.u.
      Pd    0.480    0.242   -2.238
      P     0.694   -1.459   -3.897
      N    -2.640   -2.130   -1.358
      N    -1.585   -1.837   -0.561
      C     1.848    0.508   -0.362
      C     2.761   -0.081   -1.203
      C    -2.728   -1.443   -2.663
      C    -2.198   -2.351   -3.731
      C    -0.827   -2.416   -4.245
      C    -1.634   -2.740    0.429
      C    -2.710   -3.637    0.258
      C    -3.335   -3.215   -0.903
      C     3.328   -1.430   -1.098
      C     4.446   -1.744   -1.891
      C     5.062   -2.991   -1.805
      C     4.567   -3.954   -0.924
      C     3.459   -3.652   -0.121
      C     2.848   -2.406   -0.205
      C     1.757   -2.988   -3.734
      C     1.331   -0.710   -5.473
      C     2.867   -3.220   -4.559
      C     3.515   -4.457   -4.538
      C     1.324   -4.007   -2.867
      C     3.062   -5.474   -3.696
      C     1.969   -5.244   -2.857
      C     1.258   -1.309   -6.741
      C     1.789   -0.663   -7.857
      C     1.975    0.530   -5.351
      C     2.424    0.575   -7.724
      C     2.525    1.167   -6.465
      Si   -0.825    1.913   -3.148
```

H	-4.211	-3.599	-1.411
H	-3.026	-4.449	0.902
H	-2.058	-0.579	-2.556
H	-0.145	1.525	-1.488
C	-0.765	-3.620	-5.038
C	-2.880	-3.520	-4.189
C	-0.585	-2.666	1.501
C	-4.143	-0.929	-2.884
H	3.289	0.568	-1.908
H	1.797	1.590	-0.290
H	1.404	-0.053	0.458
H	4.822	-0.997	-2.594
H	5.916	-3.219	-2.442
H	5.029	-4.939	-0.873
H	3.060	-4.403	0.562
H	1.973	-2.187	0.405
H	0.786	-2.275	-6.885
H	4.379	-4.622	-5.182
H	3.565	-6.440	-3.686
H	0.469	-3.836	-2.211
H	1.620	-6.025	-2.181
H	3.226	-2.438	-5.228
H	1.701	-1.133	-8.836
H	2.018	1.011	-4.371
H	2.831	1.075	-8.601
H	3.007	2.136	-6.346
Cl	0.225	3.753	-3.258
Cl	-1.375	1.644	-5.177
Cl	-2.706	2.400	-2.307
Fe	-2.259	-2.487	-5.774
C	-1.940	-1.043	-7.192
C	-3.990	-2.017	-6.707
C	2.636	-2.345	4.381
C	-0.093	-5.160	1.182
C	1.155	-3.690	2.828
C	-3.198	-0.835	-6.535
C	0.155	-3.802	1.856
C	1.469	-2.450	3.392
C	0.712	-1.327	3.042
C	-0.349	-1.439	2.136
C	-2.010	-4.329	-4.989
C	-1.252	-0.227	1.858
C	-3.227	-2.952	-7.480
C	-1.959	-2.352	-7.778
H	-0.948	-5.653	1.666

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      H     2.895   -1.299    4.602
      H     1.702   -4.571    3.149
      H     2.356   -2.847    5.320
      H    -1.160   -0.301   -7.316
      H    -4.998   -2.168   -6.334
      H    -0.302   -5.032    0.109
      H     0.786   -5.816    1.272
      H     0.122   -4.026   -5.512
      H     3.522   -2.841    3.958
      H    -3.536    0.093   -6.088
      H     0.948   -0.363    3.479
      H    -4.188   -0.314   -3.793
      H    -2.308   -0.539    1.863
      H    -4.449   -0.306   -2.028
      H    -2.242   -5.281   -5.456
      H    -1.129    0.552    2.625
      H    -3.901   -3.789   -3.945
      H    -4.864   -1.753   -2.984
      H    -1.016    0.212    0.878
      H    -3.554   -3.940   -7.790
      H    -1.175   -2.794   -8.384
      XX   -1.734   -3.240   -4.440
      XX   -2.860   -1.841   -7.133


Complex 13a' E=-367.02101 a.u.

      Pd    0.902    0.328   -2.423
      P     0.441   -1.283   -4.110
      N    -2.863   -1.901   -1.551
      N    -1.799   -1.579   -0.780
      C     2.544    2.793   -1.065
      C     1.919    1.426   -0.899
      C    -3.004   -1.219   -2.854
      C    -2.495   -2.126   -3.937
      C    -1.124   -2.191   -4.451
      C    -1.806   -2.473    0.218
      C    -2.865   -3.397    0.078
      C    -3.524   -2.998   -1.074
      C     2.760    0.232   -1.013
      C     4.074    0.232   -1.564
      C     4.800   -0.944   -1.667
      C     4.249   -2.170   -1.252
      C     2.956   -2.208   -0.745
      C     2.209   -1.026   -0.637
```

C	1.529	-2.776	-3.873
C	1.078	-0.591	-5.721
C	2.810	-2.838	-4.438
C	3.615	-3.964	-4.242
C	1.080	-3.849	-3.084
C	3.152	-5.040	-3.482
C	1.883	-4.975	-2.899
C	0.951	-1.201	-6.978
C	1.503	-0.607	-8.115
C	1.802	0.609	-5.635
C	2.213	0.591	-8.016
C	2.371	1.193	-6.768
Si	-0.438	2.069	-3.037
H	-4.400	-3.407	-1.562
H	-3.149	-4.210	0.734
H	-2.357	-0.338	-2.780
H	3.051	2.917	-2.030
C	-1.071	-3.385	-5.261
C	-3.196	-3.262	-4.440
C	-0.721	-2.366	1.255
C	-4.437	-0.736	-3.025
H	1.218	1.378	-0.059
H	3.286	2.973	-0.269
H	1.787	3.581	-0.999
H	4.521	1.174	-1.879
H	5.812	-0.918	-2.071
H	4.833	-3.085	-1.332
H	2.518	-3.151	-0.425
H	1.224	-1.049	-0.176
H	0.425	-2.140	-7.106
H	4.606	-3.999	-4.693
H	3.777	-5.921	-3.341
H	0.095	-3.807	-2.618
H	1.513	-5.805	-2.297
H	3.179	-2.012	-5.044
H	1.375	-1.090	-9.083
H	1.910	1.091	-4.661
H	2.640	1.050	-8.907
H	2.923	2.127	-6.671
Cl	0.406	3.984	-3.401
Cl	-1.529	1.783	-4.843
Cl	-1.982	2.466	-1.635
Fe	-2.542	-2.172	-5.976
C	-2.175	-0.664	-7.315
C	-4.260	-1.574	-6.856

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      C     2.526   -1.933    4.094
      C    -0.199   -4.855    0.950
      C     1.057   -3.356    2.561
      C    -3.414   -0.439   -6.629
      C     0.041   -3.488    1.608
      C     1.365   -2.106    3.108
      C     0.598   -0.994    2.748
      C    -0.469   -1.123    1.852
      C    -2.337   -4.058   -5.265
      C    -1.352    0.094    1.539
      C    -3.549   -2.496   -7.692
      C    -2.261   -1.934   -7.977
      H    -1.022   -5.367    1.470
      H     3.178   -1.114    3.753
      H     1.616   -4.230    2.877
      H     2.121   -1.681    5.086
      H    -1.366    0.052   -7.402
      H    -5.269   -1.702   -6.478
      H    -0.450   -4.741   -0.114
      H     0.700   -5.488    1.010
      H    -0.174   -3.825   -5.681
      H     3.133   -2.846    4.181
      H    -3.701    0.476   -6.125
      H     0.838   -0.025    3.172
      H    -4.538   -0.150   -3.948
      H    -2.414   -0.197    1.532
      H    -4.714   -0.093   -2.174
      H    -2.580   -4.997   -5.752
      H    -1.226    0.890    2.288
      H    -4.222   -3.524   -4.205
      H    -5.146   -1.574   -3.067
      H    -1.083    0.499    0.553
      H    -3.923   -3.448   -8.054
      H    -1.512   -2.367   -8.632
      XX   -2.042   -2.996   -4.673
      XX   -3.128   -1.424   -7.289

Complex 13c' E=-367.02372 a.u.

      Pd    1.112   -0.077   -1.921
      P     0.727   -1.589   -3.725
      N    -2.611   -2.228   -1.331
      N    -1.698   -1.824   -0.419
      C     1.615    1.532    0.806
      C     2.223    0.998   -0.475
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C	-2.702	-1.492	-2.609
C	-2.198	-2.351	-3.731
C	-0.827	-2.416	-4.245
C	-1.756	-2.739	0.559
C	-2.696	-3.751	0.267
C	-3.230	-3.387	-0.959
C	2.902	-0.307	-0.478
C	4.008	-0.556	-1.339
C	4.628	-1.800	-1.372
C	4.159	-2.846	-0.568
C	3.053	-2.642	0.259
C	2.426	-1.398	0.300
C	1.693	-3.157	-3.451
C	1.517	-0.851	-5.239
C	2.882	-3.453	-4.132
C	3.541	-4.665	-3.902
C	1.186	-4.082	-2.523
C	3.020	-5.590	-2.996
C	1.843	-5.292	-2.303
C	1.442	-1.375	-6.540
C	2.097	-0.744	-7.599
C	2.286	0.306	-5.034
C	2.853	0.410	-7.380
C	2.951	0.930	-6.090
Si	-0.014	1.829	-2.422
H	-3.991	-3.861	-1.567
H	-2.987	-4.603	0.869
H	-2.036	-0.631	-2.483
H	0.974	2.398	0.610
C	-0.790	-3.560	-5.120
C	-2.933	-3.409	-4.347
C	-0.849	-2.553	1.744
C	-4.124	-0.976	-2.782
H	2.786	1.767	-1.015
H	2.417	1.857	1.490
H	1.011	0.789	1.337
H	4.388	0.262	-1.952
H	5.484	-1.961	-2.027
H	4.647	-3.819	-0.599
H	2.675	-3.456	0.875
H	1.577	-1.241	0.960
H	0.876	-2.271	-6.763
H	4.460	-4.888	-4.442
H	3.529	-6.538	-2.828
H	0.269	-3.858	-1.979

H	1.431	-6.006	-1.589
H	3.289	-2.746	-4.853
H	2.012	-1.161	-8.602
H	2.345	0.729	-4.028
H	3.358	0.900	-8.211
H	3.532	1.832	-5.901
Cl	1.190	3.554	-2.747
Cl	-1.176	1.764	-4.202
Cl	-1.436	2.480	-0.993
Fe	-2.185	-2.229	-5.777
C	-1.677	-0.634	-6.950
C	-3.825	-1.468	-6.678
C	1.896	-1.872	5.030
C	-0.070	-4.984	1.526
C	0.800	-3.397	3.298
C	-2.938	-0.405	-6.308
C	-0.050	-3.608	2.206
C	0.907	-2.134	3.887
C	0.098	-1.092	3.423
C	-0.806	-1.303	2.377
C	-2.083	-4.173	-5.212
C	-1.748	-0.169	1.942
C	-3.116	-2.349	-7.560
C	-1.789	-1.833	-7.729
H	-0.906	-5.574	1.928
H	2.457	-0.947	4.830
H	1.386	-4.222	3.691
H	1.335	-1.757	5.969
H	-0.823	0.034	-6.917
H	-4.857	-1.577	-6.360
H	-0.182	-4.884	0.436
H	0.866	-5.533	1.711
H	0.107	-4.020	-5.517
H	2.616	-2.696	5.144
H	-3.202	0.471	-5.727
H	0.177	-0.114	3.886
H	-4.215	-0.386	-3.704
H	-2.770	-0.558	1.811
H	-4.390	-0.331	-1.929
H	-2.348	-5.065	-5.771
H	-1.788	0.636	2.692
H	-3.976	-3.640	-4.166
H	-4.848	-1.802	-2.823
H	-1.402	0.260	0.992
H	-3.516	-3.246	-8.022

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     H    -1.025   -2.251   -8.376
     XX   -1.763   -3.174   -4.531
     XX   -2.667   -1.340   -7.042


     Transition States

     Model A

     TS1 E=-293.84550 a.u.
Pd          0.0392     -0.0493     -0.1091
Si          1.0216     -0.1323      2.0072
Cl         -0.2556     -0.6805      3.6035
Cl          1.8972      1.6927      2.6457
Cl          2.6508     -1.5026      2.2343
P           1.2182     -1.7667     -1.0659
N           1.6874      1.5955     -3.8462
N           2.7442      1.8470     -3.0303
C           2.8346     -1.5068     -1.8811
C           3.4306     -0.3399     -2.1552
C           2.9375      1.0413     -1.8238
C           1.8310      2.4602     -4.8613
C           2.9817      3.2620     -4.7087
C           3.5482      2.8353     -3.5188
C          -1.5649      1.3274     -0.9095
C          -1.1663      0.3974     -1.9260
C          -1.9662     -0.7561     -2.3739
C          -3.0535     -1.2808     -1.6466
C          -3.7908     -2.3565     -2.1392
C          -3.4628     -2.9410     -3.3670
C          -1.6417     -1.3644     -3.6049
C          -2.3809     -2.4401     -4.0959
H          -0.4330      0.7546     -2.6529
H           0.5310     -2.4864     -2.0844
H           3.3327     -2.4281     -2.1893
H           1.0942      2.4756     -5.6578
H           4.3853     -0.3705     -2.6895
H           3.6721      1.5660     -1.1976
H           1.5360     -2.8610     -0.2246
H          -0.9071      1.1698      0.4527
H           1.9877      1.0070     -1.2652
H           3.3406      4.0476     -5.3618
H           4.4376      3.1556     -2.9884
H          -2.5628      1.2454     -0.4817
H          -1.2200      2.3540     -1.0261
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H	-3.3286	-0.8495	-0.6845
H	-4.6323	-2.7390	-1.5633
H	-4.0460	-3.7757	-3.7541
H	-0.8078	-0.9650	-4.1837
H	-2.1140	-2.8822	-5.0554

TS2 E=-293.83638 a.u.

Pd	-0.0812	-0.1820	0.0754
Si	0.7844	1.2907	1.5932
Cl	0.5008	0.6253	3.5779
Cl	1.1545	3.3961	1.7146
Cl	2.8961	0.7877	1.3619
P	1.3255	-1.8877	-0.4370
N	1.5282	1.3937	-4.3550
N	2.4356	1.5910	-3.3657
C	2.3331	-1.8336	-1.9611
C	2.7290	-0.7274	-2.6071
C	2.4589	0.6972	-2.2153
C	1.7399	2.4019	-5.2127
C	2.7792	3.2518	-4.7758
C	3.2042	2.6973	-3.5794
C	-2.0607	0.8346	-0.0850
C	-1.1508	1.6417	0.8427
C	-1.9296	2.0409	2.1192
C	-2.8043	-0.2886	0.3708
C	-3.7102	-0.9362	-0.4741
C	-3.9135	-0.4814	-1.7781
C	-3.1873	0.6184	-2.2452
C	-2.2667	1.2619	-1.4200
H	-0.8716	2.5481	0.2967
H	0.7585	-3.1832	-0.5835
H	2.6260	-2.8066	-2.3599
H	1.1275	2.4803	-6.1051
H	3.3247	-0.8447	-3.5158
H	3.2335	1.0645	-1.5269
H	2.2954	-2.2231	0.5422
H	-1.3695	2.7473	2.7399
H	1.5008	0.7725	-1.6666
H	3.1679	4.1391	-5.2575
H	3.9747	2.9938	-2.8775
H	-2.1877	1.1737	2.7344
H	-2.8611	2.5268	1.7938
H	-2.6993	-0.6263	1.4013

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H          -4.2702     -1.7939     -0.1037
H          -4.6338     -0.9750     -2.4286
H          -1.7129      2.1243     -1.7917
H          -3.3391      0.9815     -3.2601

     TS3   E=-293.76467 a.u.
Pd          0.0675     -0.0965     -0.2463
P           1.2291     -1.7631     -1.0023
N           1.6961      1.6272     -3.7472
N           2.8123      1.8212     -2.9995
C           2.8341     -1.5308     -1.8463
C           3.4640     -0.3872     -2.1415
C           3.0281      1.0115     -1.7978
C           1.8310      2.4660     -4.7840
C           3.0365      3.1949     -4.7141
C           3.6460      2.7496     -3.5521
C          -1.4551      1.6284     -1.5900
C          -0.9490      0.2411     -2.0593
C          -1.9151     -0.8096     -2.4317
C          -3.0452     -1.1438     -1.6525
C          -3.9105     -2.1696     -2.0346
C          -3.6858     -2.8911     -3.2113
C          -1.6995     -1.5623     -3.6114
C          -2.5713     -2.5809     -3.9964
Si         -1.8961      2.5455      0.0267
H          -0.2141      0.4162     -2.8482
H           0.5694     -2.5707     -1.9713
H           3.2910     -2.4701     -2.1690
H           1.0500      2.5123     -5.5359
H           4.4008     -0.4544     -2.7021
H           3.8061      1.5136     -1.2068
H           1.5779     -2.7890     -0.0893
H           0.7175     -0.1379      1.2562
H           2.0992      0.9992     -1.2030
H           3.4082      3.9407     -5.4054
H           4.5840      3.0213     -3.0817
H          -2.4905      1.7737     -1.9955
H          -0.8256      2.3911     -2.0855
H          -3.2423     -0.6005     -0.7283
H          -4.7765     -2.4019     -1.4151
H          -4.3770     -3.6753     -3.5193
H          -0.8491     -1.3155     -4.2493
H          -2.3955     -3.1174     -4.9290
Cl         -3.7200      1.8867      0.8063
Cl         -2.1774      4.5001     -0.6904
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Cl        -0.5850      2.7626      1.6633

     Model B

     TS1 E=-293.79110 a.u.
     Pd     0.635     0.209    -2.251
     P      0.733    -1.470    -3.826
     N     -2.512    -2.235    -1.279
     N     -1.494    -1.872    -0.463
     C      1.746     0.492    -0.362
     C      2.194    -0.736    -0.930
     C     -2.622    -1.547    -2.584
     C     -2.066    -2.457    -3.636
     C     -0.695    -2.522    -4.150
     C     -1.484    -2.787     0.515
     C     -2.483    -3.765     0.319
     C     -3.124    -3.378    -0.845
     C      3.480    -0.898    -1.646
     C      3.988     0.104    -2.497
     C      5.154    -0.097    -3.230
     C      5.874    -1.290    -3.101
     C      5.416    -2.272    -2.221
     C      4.225    -2.087    -1.512
     Si    -0.618     1.847    -3.350
     H     -3.964    -3.824    -1.364
     H     -2.739    -4.609     0.948
     H     -1.983    -0.660    -2.482
     H      0.657     1.372    -1.147
     C      1.934    -2.848    -3.501
     C      1.385    -0.822    -5.449
     C     -0.594    -3.769    -4.859
     C     -2.731    -3.648    -4.069
     C     -0.440    -2.628     1.583
     C     -4.050    -1.078    -2.812
     H      1.777    -1.652    -0.508
     H      2.431     1.340    -0.358
     H      1.101     0.430     0.512
     H      3.437     1.038    -2.606
     H      5.496     0.677    -3.915
     H      6.781    -1.449    -3.683
     H      5.981    -3.197    -2.100
     H      3.873    -2.872    -0.842
     Cl     0.252     3.783    -3.318
     Cl    -0.918     1.564    -5.439
     Cl    -2.595     2.196    -2.656
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Fe	-2.092	-2.662	-5.671
C	-1.738	-1.277	-7.143
C	3.138	-2.985	-4.200
C	-3.812	-2.159	-6.595
C	2.827	-1.940	4.341
C	0.252	-5.074	1.280
C	1.433	-3.471	2.853
C	-2.973	-1.004	-6.468
C	0.410	-3.688	1.923
C	3.943	-4.108	-3.992
C	1.643	-2.202	3.401
C	0.759	-1.165	3.087
C	-0.321	-1.389	2.227
C	1.603	-3.777	-2.509
C	3.590	-5.056	-3.027
C	-1.838	-4.479	-4.821
C	2.427	-4.881	-2.272
C	-1.376	-0.291	2.010
C	-3.095	-3.147	-7.347
C	-1.809	-2.605	-7.679
C	1.390	-1.565	-6.634
C	1.896	-1.018	-7.816
C	1.933	0.465	-5.460
C	2.421	0.277	-7.821
C	2.444	1.018	-6.637
H	-0.546	-5.622	1.802
H	1.006	-2.573	-6.655
H	3.248	-0.940	4.156
H	2.074	-4.293	3.151
H	2.474	-1.994	5.381
H	-0.944	-0.562	-7.321
H	4.847	-4.242	-4.577
H	-4.816	-2.264	-6.197
H	-0.003	-4.988	0.214
H	1.183	-5.657	1.352
H	0.325	-4.214	-5.224
H	3.626	-2.682	4.194
H	-3.254	-0.060	-6.014
H	0.912	-0.183	3.521
H	-4.119	-0.509	-3.750
H	-2.383	-0.730	2.074
H	4.220	-5.924	-2.862
H	0.699	-3.643	-1.924
H	-4.364	-0.425	-1.983
H	-2.048	-5.458	-5.240

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H    -1.301    0.494    2.778
H    -3.757   -3.916   -3.846
H     2.164   -5.601   -1.503
H    -4.749   -1.924   -2.865
H    -1.256    0.178    1.023
H     3.462   -2.229   -4.905
H    -3.459   -4.134   -7.614
H    -1.042   -3.099   -8.266
H     1.881   -1.599   -8.733
H     1.962    1.045   -4.546
H     2.810    0.704   -8.740
H     2.858    2.021   -6.631
XX   -1.583   -3.368   -4.307
XX   -2.684   -2.039   -7.044

TS2 E=-293.78807 a.u.
Pd    0.736    0.108   -2.896
P     0.296   -1.533   -4.447
N    -2.780   -2.259   -1.901
N    -1.705   -1.965   -1.131
C     2.263    2.922   -1.490
C     1.531    1.564   -1.513
C    -2.937   -1.536   -3.175
C    -2.517   -2.425   -4.306
C    -1.172   -2.502   -4.884
C    -1.727   -2.871   -0.145
C    -2.808   -3.768   -0.289
C    -3.464   -3.344   -1.432
C     2.535    0.426   -1.587
C     3.576    0.405   -2.555
C     4.541   -0.601   -2.547
C     4.507   -1.614   -1.583
C     3.484   -1.620   -0.631
C     2.511   -0.620   -0.633
Si   -0.198    2.148   -2.846
H    -4.351   -3.724   -1.924
H    -3.104   -4.581    0.363
H    -2.239   -0.692   -3.106
H     2.942    2.896   -0.624
C     1.471   -2.879   -3.941
C     0.967   -1.032   -6.103
C    -1.175   -3.628   -5.769
C    -3.275   -3.495   -4.874
C    -0.647   -2.810    0.901
C    -4.340   -0.964   -3.276
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H	0.947	1.460	-0.593
H	1.585	3.770	-1.363
H	2.861	3.094	-2.390
H	3.628	1.195	-3.303
H	5.328	-0.593	-3.301
H	5.272	-2.388	-1.573
H	3.447	-2.403	0.127
H	1.734	-0.614	0.128
Cl	0.690	3.592	-4.115
Cl	-2.034	1.852	-3.961
Cl	-1.075	3.193	-1.216
Fe	-2.580	-2.339	-6.362
C	-1.872	-1.336	-7.971
C	2.841	-2.751	-4.191
C	-3.955	-0.988	-7.012
C	2.532	-2.532	3.836
C	-0.175	-5.302	0.541
C	1.081	-3.876	2.215
C	-2.625	-0.461	-7.119
C	0.083	-3.958	1.237
C	3.726	-3.756	-3.794
C	1.396	-2.651	2.813
C	0.662	-1.513	2.468
C	-0.375	-1.588	1.531
C	0.995	-4.001	-3.255
C	3.246	-4.882	-3.119
C	-2.461	-4.265	-5.771
C	1.880	-5.004	-2.849
C	-1.210	-0.338	1.213
C	-4.017	-2.198	-7.778
C	-2.730	-2.412	-8.373
C	1.613	-1.924	-6.967
C	2.071	-1.486	-8.214
C	0.786	0.297	-6.496
C	1.891	-0.155	-8.600
C	1.248	0.738	-7.739
H	-0.996	-5.823	1.055
H	1.770	-2.957	-6.682
H	2.115	-2.212	4.803
H	1.619	-4.770	2.510
H	3.064	-3.484	3.978
H	-0.848	-1.194	-8.292
H	4.786	-3.661	-4.007
H	-4.791	-0.519	-6.505
H	-0.439	-5.157	-0.517

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H     0.721   -5.942    0.572
H    -0.321   -3.994   -6.325
H     3.254   -1.777    3.488
H    -2.264    0.456   -6.667
H     0.905   -0.566    2.938
H    -4.415   -0.296   -4.145
H    -2.281   -0.588    1.225
H     3.934   -5.661   -2.805
H    -0.062   -4.096   -3.029
H    -4.568   -0.379   -2.372
H    -2.757   -5.144   -6.334
H    -1.042    0.464    1.948
H    -4.305   -3.731   -4.632
H     1.507   -5.877   -2.323
H    -5.094   -1.759   -3.373
H    -0.942    0.044    0.218
H     3.221   -1.867   -4.692
H    -4.888   -2.833   -7.897
H    -2.454   -3.241   -9.016
H     2.568   -2.181   -8.883
H     0.283    0.991   -5.831
H     2.250    0.185   -9.566
H     1.106    1.773   -8.034
XX   -2.117   -3.260   -5.117
XX   -3.040   -1.477   -7.650

TS4   E=-293.76592 a.u.
Pd    0.488    0.899   -4.221
P     0.368   -1.445   -4.853
N    -2.594   -2.272   -1.976
N    -1.435   -2.134   -1.282
C     2.220    3.025   -0.831
C     1.547    1.696   -1.152
C    -2.731   -1.501   -3.229
C    -2.382   -2.391   -4.385
C    -1.078   -2.529   -5.038
C    -1.475   -3.088   -0.344
C    -2.645   -3.871   -0.448
C    -3.338   -3.322   -1.514
C     2.467    0.579   -1.526
C     3.753    0.817   -2.044
C     4.671   -0.225   -2.197
C     4.339   -1.521   -1.801
C     3.052   -1.781   -1.319
C     2.122   -0.750   -1.209
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Si	-0.213	2.320	-2.416
Si	2.207	2.468	-5.420
H	-4.295	-3.592	-1.944
H	-2.966	-4.693	0.179
H	-1.986	-0.703	-3.144
H	3.038	2.851	-0.114
C	1.646	-2.618	-4.210
C	0.944	-1.311	-6.621
C	-1.147	-3.714	-5.837
C	-3.170	-3.514	-4.794
C	-0.289	-3.193	0.572
C	-4.102	-0.852	-3.296
H	0.891	1.369	-0.339
H	1.516	3.736	-0.385
H	2.653	3.502	-1.719
H	4.054	1.828	-2.309
H	5.660	-0.015	-2.602
H	5.079	-2.318	-1.857
H	2.777	-2.789	-1.009
H	1.113	-0.969	-0.867
H	2.169	1.199	-4.339
Cl	-0.043	4.384	-2.755
Cl	-1.772	1.854	-4.049
Cl	-1.634	2.134	-0.853
Cl	3.503	3.813	-4.501
Cl	3.301	1.474	-6.889
Cl	0.804	3.608	-6.444
Fe	-2.624	-2.497	-6.415
C	-2.132	-1.698	-8.206
C	2.995	-2.409	-4.515
C	-4.059	-1.190	-7.018
C	3.488	-3.203	2.678
C	-0.047	-5.664	-0.036
C	1.640	-4.397	1.382
C	-2.752	-0.714	-7.366
C	0.441	-4.386	0.660
C	3.949	-3.360	-4.145
C	2.115	-3.233	1.995
C	1.325	-2.080	1.982
C	0.092	-2.074	1.322
C	1.274	-3.703	-3.410
C	3.568	-4.478	-3.398
C	-2.419	-4.359	-5.677
C	2.233	-4.641	-3.017
C	-0.841	-0.859	1.426

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C    -4.241   -2.474   -7.629
C    -3.052   -2.787   -8.366
C     1.621   -2.335   -7.293
C     2.005   -2.166   -8.627
C     0.649   -0.125   -7.300
C     1.719   -0.972   -9.295
C     1.039    0.051   -8.630
H    -0.865   -6.102    0.553
H     1.858   -3.267   -6.793
H     4.024   -2.284    2.397
H     2.210   -5.316    1.466
H     3.345   -3.217    3.769
H    -1.156   -1.630   -8.670
H     4.987   -3.228   -4.435
H    -4.804   -0.654   -6.442
H    -0.408   -5.442   -1.051
H     0.758   -6.411   -0.122
H    -0.345   -4.109   -6.447
H     4.105   -4.066    2.388
H    -2.328    0.240   -7.073
H     1.675   -1.188    2.490
H    -4.148   -0.160   -4.149
H    -1.854   -1.199    1.690
H     4.309   -5.218   -3.111
H     0.244   -3.821   -3.093
H    -4.287   -0.278   -2.374
H    -2.752   -5.279   -6.147
H    -0.505   -0.151    2.198
H    -4.181   -3.726   -4.466
H     1.942   -5.496   -2.415
H    -4.899   -1.601   -3.406
H    -0.885   -0.330    0.465
H     3.301   -1.512   -5.043
H    -5.126   -3.096   -7.554
H    -2.877   -3.690   -8.941
H     2.528   -2.964   -9.145
H     0.113    0.667   -6.790
H     2.024   -0.840  -10.329
H     0.812    0.980   -9.145
XX   -2.037   -3.299   -5.141
XX   -3.246   -1.770   -7.718

Model C

TS2  E=-366.98801 a.u.
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Pd	0.994	0.421	-2.493
P	0.573	-1.165	-4.187
N	-2.246	-2.161	-1.248
N	-1.299	-1.663	-0.410
C	2.597	3.201	-1.654
C	1.759	1.996	-1.196
C	-2.524	-1.440	-2.510
C	-2.168	-2.243	-3.728
C	-0.916	-2.186	-4.490
C	-1.323	-2.478	0.656
C	-2.283	-3.502	0.507
C	-2.863	-3.261	-0.727
C	2.632	0.770	-0.946
C	3.954	0.676	-1.452
C	4.788	-0.382	-1.095
C	4.327	-1.399	-0.257
C	3.016	-1.349	0.223
C	2.181	-0.280	-0.102
C	1.703	-2.630	-3.953
C	0.811	-0.302	-5.812
C	2.895	-2.880	-4.644
C	3.631	-4.040	-4.368
C	1.279	-3.544	-2.968
C	3.188	-4.956	-3.413
C	2.010	-4.700	-2.706
C	1.028	-0.908	-7.062
C	0.968	-0.142	-8.230
C	0.569	1.082	-5.770
C	0.669	1.222	-8.175
C	0.481	1.838	-6.938
Si	-0.262	2.266	-2.117
H	-3.658	-3.780	-1.249
H	-2.547	-4.286	1.206
H	-1.879	-0.556	-2.469
H	2.058	4.141	-1.541
C	-0.937	-3.293	-5.397
C	-2.900	-3.368	-4.226
C	-0.338	-2.293	1.780
C	-3.968	-0.958	-2.471
H	1.242	2.213	-0.255
H	2.906	3.122	-2.703
H	3.504	3.254	-1.034
H	4.340	1.457	-2.102
H	5.810	-0.407	-1.473
H	4.982	-2.225	0.018

H	2.643	-2.145	0.866
H	1.171	-0.233	0.302
H	1.246	-1.972	-7.141
H	4.556	-4.230	-4.913
H	3.760	-5.862	-3.216
H	0.365	-3.353	-2.405
H	1.657	-5.400	-1.952
H	3.253	-2.180	-5.398
H	1.139	-0.623	-9.193
H	0.406	1.560	-4.806
H	0.585	1.800	-9.094
H	0.246	2.899	-6.872
Cl	0.003	4.199	-2.973
Cl	-2.084	1.854	-3.252
Cl	-1.205	2.639	-0.248
Fe	-2.534	-2.138	-5.764
C	-2.334	-1.629	-7.707
C	-3.709	-0.516	-6.206
C	2.564	-1.862	4.982
C	0.472	-4.689	1.354
C	1.388	-3.225	3.201
C	-2.461	-0.447	-6.905
C	0.496	-3.364	2.132
C	1.527	-2.002	3.861
C	0.714	-0.929	3.481
C	-0.243	-1.077	2.471
C	-2.148	-4.047	-5.241
C	-1.157	0.124	2.188
C	-4.351	-1.746	-6.565
C	-3.506	-2.430	-7.500
H	-0.316	-5.338	1.762
H	2.614	-0.835	5.374
H	1.987	-4.071	3.523
H	2.299	-2.542	5.805
H	-1.507	-1.867	-8.367
H	-4.143	0.283	-5.616
H	0.289	-4.518	0.283
H	1.436	-5.214	1.441
H	-0.120	-3.587	-6.044
H	3.557	-2.137	4.594
H	-1.788	0.399	-6.903
H	0.821	0.029	3.979
H	-4.187	-0.315	-3.333
H	-1.722	0.358	3.102
H	-4.142	-0.375	-1.553

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H    -2.432   -4.948   -5.776
H    -0.530    0.990    1.932
H    -3.865   -3.701   -3.859
H    -4.671   -1.803   -2.480
H    -1.878   -0.043    1.377
H    -5.319   -2.087   -6.212
H    -3.714   -3.387   -7.967
XX   -1.813   -3.022   -4.615
XX   -3.270   -1.355   -6.974
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