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Electronic Effects on the Stability of Isomeric Alkyl-Metal Compounds

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Supplementary Information

Shown below are the optimized geometries (Cartesian coordinates in Å) and total energies (in Hartrees) for all the species discussed in this paper. The format is:
Formula; number of basis functions; total energy; (*where applicable:* number of basis functions with BSII, total energy for BSII single-point calculation); Cartesian coordinates.
The ASCII file containing these coordinates can be obtained upon request from the author.

A. Hydrocarbon Reference Compounds.

CH4 34 -40.523249
(50 -40.533339)
C 0.0000 0.0000 0.0000
H 0.6305 -0.6305 -0.6305
H 0.6305 0.6305 0.6305
H -0.6305 0.6305 -0.6305
H -0.6305 -0.6305 0.6305

C3H8 82 -119.153059
(122 -119.180717)
C 0.0000 0.0000 0.5780
C 0.0000 1.2767 -0.2691
C 0.0000 -1.2767 -0.2691
H 0.8768 0.0000 1.2383
H -0.8768 0.0000 1.2383
H 0.0000 2.1755 0.3564
H -0.8838 1.3204 -0.9160
H 0.8838 -1.3204 -0.9160
H -0.8838 -1.3204 -0.9160
H 0.0000 -2.1755 0.3564
H 0.8838 1.3204 -0.9160

HC(CH3)3 106 -158.469784
(158 -158.505194)
C 0.0000 0.0000 0.3651
C 1.4620 0.0000 -0.1047
C -0.7310 -1.2661 -0.1047
H 0.0000 0.0000 1.4649
C -0.7310 1.2661 -0.1047
H 1.9977 0.8855 0.2550
H 1.5185 0.0000 -1.2004
H -1.7657 1.2874 0.2550
H -0.2320 2.1728 0.2550
H -0.7593 1.3151 -1.2004
H -0.2320 -2.1728 0.2550
H -0.7593 -1.3151 -1.2004
H -1.7657 -1.2874 0.2550
H 1.9977 -0.8855 0.2550

CH3CH2CN 81 -172.071493
(123 -172.119989)
C 0.7659 0.4653 0.0000
C -0.1103 1.7313 0.0000
C -0.0279 -0.7670 0.0000
H 1.4199 0.4501 -0.8796
H 1.4199 0.4501 0.8796
H 0.5255 2.6207 0.0000
H -0.7503 1.7628 0.8854
H -0.7503 1.7628 -0.8854
N -0.6721 -1.7323 0.0000

CH3CH2CF3 121 -416.899256
(167 -417.010906)
C 1.2379 0.3068 0.0000
C 1.2386 1.8385 0.0000
C -0.1503 -0.2961 0.0000
H 1.7518 -0.0877 -0.8822
H 1.7518 -0.0877 0.8822
H 2.2683 2.2057 0.0000
H 0.7376 2.2362 0.8864
H 0.7376 2.2362 -0.8864
F -0.8751 0.0709 -1.0902
F -0.8751 0.0709 1.0902
F -0.1036 -1.6548 0.0000

B. Alkyllithium.

CH3Li 43 -47.405207
C 0.0000 0.0000 0.5709
H 1.0165 0.0000 0.9915
H -0.5082 0.8803 0.9915
H -0.5082 -0.8803 0.9915

CH3CH2CH2Li 91 -126.030095
C 0.0000 0.0000 0.0000
C 0.0000 0.0000 1.5411
H 1.0337 0.0000 -0.3798
C -0.7446 1.1850 -0.6405
H 0.5458 -0.8938 1.8913
H 0.4324 0.9536 1.8914
H -0.7225 1.1503 -1.7386
H -1.7953 1.1974 -0.3262
H -0.3001 2.1370 -0.3259

CH3CHLiCH3 91 -126.024203
C -0.0041 0.0243 0.0267
C -0.0165 0.0698 1.5647
H 1.0137 0.0614 -0.3849
H -0.4709 -0.8925 -0.3631
H -0.5618 0.8646 -0.4304
C -1.4648 0.1753 2.0743
H 0.4972 1.0007 1.8626
H -1.5164 0.3234 3.1616
H -2.0203 1.0151 1.6133
H -2.0486 -0.7295 1.8490

(CH3)2CHCH2Li
115 -165.347268
C 0.0095 -0.0033 -0.0055
C -0.0325 -0.0021 1.5370
C 1.4508 -0.0224 -0.5401
H -0.4831 -0.9208 -0.3679
C -0.7512 1.1882 -0.6239
H -1.0860 -0.0041 1.8628
H 0.3660 0.9674 1.8895
H -0.7550 1.1588 -1.7226
H -1.7923 1.2040 -0.2837
H -0.2911 2.1362 -0.3162
H 1.9908 -0.9186 -0.2024
H 2.0075 0.8516 -0.1772
H 1.4895 -0.0069 -1.6366

(CH3)3CLi 115 -165.338753
C 0.0000 -1.4379 -0.3627
C 0.0000 0.0000 0.1822
H 0.8849 -2.0071 -0.0449
H -0.8849 -2.0071 -0.0449
H 0.0000 -1.4546 -1.4730
C -1.2452 0.7189 -0.3627
C 1.2452 0.7189 -0.3627
H -1.2957 1.7699 -0.0449
H -1.2597 0.7273 -1.4730
H -2.1806 0.2372 -0.0449
H 1.2597 0.7273 -1.4730
H 2.1806 0.2372 -0.0449
H 1.2957 1.7699 -0.0449

C. Zirconocenes

Cp2Zr(H)CH3
225 -474.206146
Zr 0.0087 0.0076 -0.0015
C -0.0165 -0.0123 2.5676
C 1.3479 -0.0229 2.1698
C 1.6376 1.2324 1.5688
C 0.4507 2.0039 1.5705
C -0.5730 1.2347 2.1891
H -0.5375 -0.8199 3.0628
H 2.0506 -0.8321 2.3262
H 2.5975 1.5404 1.1742
H 0.3350 3.0003 1.1632
H -1.5967 1.5509 2.3373
C 0.3858 0.7081 -2.4583
C 1.6198 0.8616 -1.7785
C 2.0795 -0.4333 -1.4000
C 1.1297 -1.3835 -1.8590
C 0.0795 -0.6783 -2.4959
H -0.2209 1.5038 -2.8675
H 2.1303 1.7977 -1.5908
H 3.0077 -0.6558 -0.8885
H 1.1850 -2.4555 -1.7230
H -0.8122 -1.1173 -2.9250
H -1.4504 1.0709 -0.4702
C -0.9628 -2.0221 0.4170
H -0.2980 -2.7436 0.9120
H -1.8199 -1.8669 1.0881
H -1.3379 -2.4966 -0.4976

273 -552.832090
Zr 0.0898 -0.0503 0.0291
C 0.0267 0.0093 2.5996
C 1.3927 0.1038 2.2218
C 1.5826 1.3588 1.5822
C 0.3338 2.0246 1.5411
C -0.6297 1.1905 2.1712
H -0.4309 -0.8219 3.1182
H 2.1595 -0.6366 2.4139
H 2.5190 1.7356 1.1912
H 0.1401 2.9934 1.0984
H -1.6796 1.4204 2.2940
C 0.4935 0.6392 -2.4325
C 1.6908 0.8909 -1.7183
C 2.2279 -0.3615 -1.3016
C 1.3634 -1.3846 -1.7730
C 0.2878 -0.7657 -2.4555
H -0.1576 1.3827 -2.8709
H 2.1277 1.8637 -1.5323
H 3.1528 -0.5094 -0.7580
H 1.4940 -2.4477 -1.6210
H -0.5564 -1.2727 -2.9057
H -1.4601 0.8472 -0.4987
C 0.1578 -3.2512 1.1736
C -0.6843 -2.1595 0.4970
H 1.0515 -3.4596 0.5676
H 0.5372 -2.8876 2.1389
C -0.5931 -4.5714 1.4080
H -1.5745 -1.9526 1.1185
H -1.0728 -2.5480 -0.4583
H 0.0446 -5.3225 1.8903
H -1.4695 -4.4140 2.0474
H -0.9500 -4.9919 0.4607

Cp2Zr(H)CH(CH3)2
273 -552.826629
Zr 0.0370 -0.0736 0.0502
C 0.0552 0.0386 2.6238
C 1.4021 0.1000 2.1765
C 1.5819 1.3412 1.5012
C 0.3476 2.0363 1.5224
C -0.5945 1.2276 2.2100
H -0.3954 -0.7751 3.1760
H 2.1665 -0.6467 2.3516
H 2.5032 1.6976 1.1588
H 0.1529 3.0060 1.0859
H -1.6340 1.4749 2.3775
C 1.5780 0.0571 -2.0243
C 2.3125 -0.6221 -1.0240
C 1.6662 -1.8633 -0.7671
C 0.5477 -1.9588 -1.6364
C 0.4832 -0.7676 -2.4010
H 1.7959 1.0399 -2.4217
H 3.2086 -0.2617 -0.5360
H 1.9933 -2.6190 -0.0636
H -0.1391 -2.7917 -1.6958
H -0.2672 -0.5206 -3.1405
C -1.4662 -2.9127 1.0876
C -1.7170 -1.5430 0.4435
H -0.6805 -3.4821 0.5777
H -1.1573 -2.8109 2.1364
H -2.3719 -3.5403 1.0894
C -2.9175 -0.8453 1.1073
H -2.0050 -1.7180 -0.6097
H -3.1186 0.1476 0.6849
H -3.8405 -1.4337 0.9818
H -2.7696 -0.7204 2.1870

Cp2Zr(H)CH2CH(CH3)2
297 -592.147279
Zr 0.0923 -0.0371 0.0215
C 0.0579 -0.0035 2.5999
C 1.4209 0.0923 2.2090
C 1.6013 1.3420 1.5612
C 0.3487 2.0077 1.5315
C -0.6050 1.1769 2.1802
H -0.3941 -0.8367 3.1206
H 2.1868 -0.6526 2.3846
H 2.5328 1.7196 1.1595
H 0.1496 2.9758 1.0899
H -1.6497 1.4119 2.3296
C 1.1998 0.8935 -2.3853
C 2.1329 0.0384 -1.4812
C 1.3651 -1.0475 -1.9786
C 0.1644 -0.5215 -2.5157
H -0.5709 1.5793 -2.7092
H 1.7402 2.2439 -1.5033
H 3.1101 -0.0315 -1.0199
H 1.6387 -2.0922 -1.9305
H -0.6453 -1.0956 -2.9484
H -1.6092 0.6497 -0.3201
C 0.3857 -3.2634 1.3161
C -0.3439 -2.2456 0.4250
C 1.7503 -3.6535 0.7261
H 2.3989 -2.7792 0.6028
H 1.6275 -4.1189 -0.2604
H 2.2712 -4.3749 1.3664
H 0.5749 -2.8013 2.2964
C -0.4611 -4.5259 1.5667
H -1.3440 -2.0327 0.8634
H -0.5499 -2.7162 -0.5490
H 0.0554 -5.2357 2.2251
H -1.4207 -4.2725 2.0305
H -0.6760 -5.0409 0.6221

Cp2Zr(H)C(CH3)3
297 -592.135545
Zr 0.0263 -0.0624 0.0376
C 0.0439 0.0317 2.6160
C 1.3932 0.0819 2.1767
C 1.5892 1.3264 1.5135
C 0.3621 2.0323 1.5299
C -0.5923 1.2302 2.2075
H -0.4123 -0.7782 3.1678
H 2.1485 -0.6732 2.3532
H 2.5177 1.6797 1.0861
H 0.1818 3.0101 1.1052
H -1.6277 1.4924 2.3755
C 1.2055 0.1112 -2.2665
C 2.2128 -0.0848 -1.2913
C 2.0498 -1.3885 -0.7421
C 0.9475 -2.0001 -1.3956
C 0.4222 -1.0705 -2.3269
H 1.0587 1.0009 -2.8629
H 2.9822 0.6265 -1.0234
H 2.6800 -1.8481 0.0083
H 0.5797 -3.0003 -1.2137
H -0.4312 -1.2269 -2.9719
H -0.7714 1.3569 -0.8684
C -1.3939 -2.9297 1.1727
C -1.7287 -1.6247 0.4348
H -0.6507 -3.5334 0.6386
H -1.0025 -2.7525 2.1814
H -2.2929 -3.5603 1.2871
C -2.8347 -0.8834 1.2209
C -2.3501 -1.9801 -0.9356
H -3.0787 0.0963 0.7886
H -3.7687 -1.4708 1.2043
H -2.5776 -0.7305 2.2728
H -3.3112 -2.5027 -0.7914
H -1.7156 -2.6451 -1.5285
H -2.5702 -1.0934 -1.5453

Cp2Zr(Cl)CH3
242 -933.894467
Zr -0.0101 0.0141 -0.0100
C 0.1984 -0.2053 2.5512
C 1.4982 0.0681 2.0514
C 1.4977 1.3938 1.5311
C 0.1963 1.9274 1.6980
C -0.6088 0.9366 2.3209
H -0.1218 -1.1279 3.0144
H 2.3475 -0.6020 2.0885
H 2.3458 1.9076 1.0978
H -0.1384 2.9059 1.3783
H -1.6612 1.0331 2.5527
C 0.7192 0.4508 -2.4508
C 1.8717 0.5788 -1.6351
C 2.1773 -0.7091 -1.1051
C 1.2064 -1.6216 -1.5878
C 0.2991 -0.9018 -2.4095
H 0.2184 1.2526 -2.9765
H 2.4380 1.4867 -1.4734
H 3.0162 -0.9504 -0.4654
H 1.1587 -2.6781 -1.3624
H -0.5752 -1.3080 -2.9012
Cl -2.0565 1.1840 -0.7517
C -0.9689 -2.0059 0.4697
H -0.2898 -2.7542 0.8960
H -1.7847 -1.8470 1.1853
H -1.3997 -2.4259 -0.4467

Cp2Zr(Cl)CH2CH2CH3
290 -1012.519990
Zr 0.0626 0.0865 -0.0155
C 0.0621 -0.0312 2.5735
C 1.4050 0.2136 2.1773
C 1.4606 1.5087 1.6017
C 0.1493 2.0511 1.6101
C -0.7123 1.0995 2.2240
H -0.3037 -0.9310 3.0484
H 2.2401 -0.4631 2.3067
H 2.3482 1.9949 1.2192
H -0.1441 3.0217 1.2297
H -1.7784 1.2117 2.3644
C 0.5581 0.9364 -2.4028
C 1.6858 1.2484 -1.6047
C 2.3055 0.0224 -1.2230
C 1.5569 -1.0395 -1.7908
C 0.4694 -0.4752 -2.5063
H -0.1414 1.6467 -2.8231
H 2.0267 2.2433 -1.3493
H 3.2028 -0.0793 -0.6257
H 1.7736 -2.0937 -1.6899
H -0.3078 -1.0228 -3.0232
Cl -2.2805 0.5684 -0.6491
C 0.8406 -3.0707 1.0252
C -0.2206 -2.1557 0.4010
H 1.7640 -3.0438 0.4290
H 1.1219 -2.6965 2.0188
C 0.3898 -4.5337 1.1640
H -1.1212 -2.1605 1.0361
H -0.5381 -2.5736 -0.5662
H 1.1703 -5.1571 1.6165
H -0.5062 -4.6086 1.7906
H 0.1423 -4.9620 0.1860

Cp2Zr(Cl)CH(CH3)2
290 -1012.514515
Zr -1.5656 -0.2448 -4.2691
C -1.2541 0.9838 -6.5083
C -0.8282 -0.3551 -6.7002
C -1.9732 -1.1980 -6.5981
C -3.0987 -0.3755 -6.3469
C -2.6551 0.9685 -6.2788
H -0.6238 1.8609 -6.5394
H 0.1838 -0.6779 -6.9090
H -1.9885 -2.2736 -6.7168
H -4.1134 -0.7154 -6.1880
H -3.2763 1.8284 -6.0680
C -1.2506 -2.5537 -3.1963
C -0.2591 -2.4559 -4.2043
C 0.6626 -1.4454 -3.8194
C 0.2547 -0.9432 -2.5554
C -0.9298 -1.6178 -2.1747
H -2.1074 -3.2156 -3.2041
H -0.2105 -3.0467 -5.1092
H 1.5358 -1.1318 -4.3780
H 0.7578 -0.1729 -1.9884
H -1.5077 -1.4389 -1.2782
Cl -3.7379 -0.0574 -3.0890
C 0.7916 2.1574 -3.9007
C -0.6598 1.7849 -3.5683
H 1.5093 1.3785 -3.6217
H 0.9252 2.3460 -4.9736
H 1.0978 3.0800 -3.3836
C -1.5905 2.9789 -3.8458
H -0.7163 1.5977 -2.4824
H -2.6337 2.7651 -3.5911
H -1.2846 3.8538 -3.2509
H -1.5605 3.2915 -4.8966

Cp2Zr(Cl)CH2CH(CH3)2
314 -1051.833537
Zr 0.0181 -0.0164 -0.0278
C -0.0296 -0.0255 2.5688
C 1.3383 -0.0989 2.1860
C 1.6799 1.1221 1.5547
C 0.5174 1.9399 1.5174
C -0.5327 1.2321 2.1652
H -0.5894 -0.8030 3.0708
H 2.0029 -0.9356 2.3567
H 2.6550 1.3847 1.1662
H 0.4491 2.9361 1.0980
H -1.5483 1.5815 2.2881
C 0.4653 0.8814 -2.4064
C 1.6627 1.0455 -1.6705
C 2.1732 -0.2509 -1.3684
C 1.2913 -1.2089 -1.9308
C 0.2269 -0.5104 -2.5551
H -0.1824 1.6744 -2.7562
H 2.1156 1.9896 -1.3962
H 3.0882 -0.4669 -0.8315
H 1.4065 -2.2813 -1.8813
H -0.6300 -0.9551 -3.0441
Cl -2.3012 0.6938 -0.5620
C 0.3022 -3.2509 1.2656
C -0.4670 -2.2198 0.4205
C 1.6466 -3.6569 0.6411
H 2.3078 -2.7950 0.5016
H 1.4951 -4.1241 -0.3404
H 2.1713 -4.3853 1.2699
H 0.5197 -2.8044 2.2469
C -0.5517 -4.5069 1.5272
H -1.4362 -2.0249 0.9148
H -0.7233 -2.6745 -0.5484
H -0.0226 -5.2283 2.1622
H -1.4942 -4.2488 2.0221
H -0.8002 -5.0096 0.5844

Cp2Zr(Cl)C(CH3)3
314 -1051.821848
Zr 0.0093 -0.0253 0.0033
C -0.1062 -0.1108 2.5809
C 1.2645 -0.1890 2.2261
C 1.6408 1.0623 1.6605
C 0.5019 1.9035 1.6633
C -0.5798 1.1776 2.2219
H -0.6801 -0.8917 3.0569
H 1.9166 -1.0366 2.3917
H 2.6283 1.3338 1.3129
H 0.4518 2.9099 1.2696
H -1.5915 1.5417 2.3353
C 1.3909 0.0451 -2.1871
C 2.2900 -0.2845 -1.1439
C 1.9380 -1.5730 -0.6510
C 0.8248 -2.0349 -1.3981
C 0.4797 -1.0299 -2.3387
H 1.3736 0.9723 -2.7443
H 3.1145 0.3261 -0.8019
H 2.4512 -2.1198 0.1291
H 0.3387 -2.9917 -1.2793
H -0.3438 -1.0646 -3.0383
Cl -1.2568 1.7655 -1.1524
C -1.5258 -2.8772 1.0261
C -1.8150 -1.5454 0.3132
H -0.7888 -3.4920 0.4996
H -1.1574 -2.7396 2.0506
H -2.4460 -3.4810 1.1024
C -2.9282 -0.8075 1.0944
C -2.4187 -1.8626 -1.0754
H -3.1707 0.1669 0.6559
H -3.8539 -1.4063 1.0710
H -2.6855 -0.6515 2.1491
H -3.3812 -2.3856 -0.9482
H -1.7869 -2.5176 -1.6816
H -2.6252 -0.9580 -1.6582

Cp2ZrCH3+
220 -473.386840
Zr 0.0101 0.0052 -0.0019
C -0.0162 -0.0122 2.5376
C 1.3467 -0.0148 2.1334
C 1.6272 1.2376 1.5126
C 0.4327 1.9988 1.5003
C -0.5871 1.2225 2.1304
H -0.5245 -0.8063 3.0667

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H  2.0615 -0.8092  2.3126
H  2.5893  1.5554  1.1330
H  0.3227  3.0050  1.1122
H -1.6084  1.5399  2.3111
C  0.4288  0.6606 -2.4261
C  1.6609  0.7864 -1.7397
C  2.0616 -0.5177 -1.3176
C  1.0860 -1.4488 -1.7792
C  0.0697 -0.7201 -2.4447
H -0.1303  1.4702 -2.8834
H  2.2107  1.7051 -1.5813
H  2.9844 -0.7642 -0.8072
H  1.1135 -2.5216 -1.6419
H -0.8123 -1.1423 -2.9114
C -1.0106 -1.9525  0.4437
H -0.4154 -2.6732  1.0169
H -1.8879 -1.7081  1.0628
H -1.3542 -2.4516 -0.4673
```

Cp2ZrCH2CH2CH3+
268 -552.029495

```
Zr  0.0085  0.0536 -0.0003
C   0.0065 -0.0924  2.5351
C   1.3583 -0.1795  2.0911
C   1.7220  1.0855  1.5390
C   0.5906  1.9363  1.6137
C  -0.4696  1.2056  2.2275
H -0.5540 -0.8763  3.0278
H   2.0173 -1.0294  2.2200
H   2.6968  1.3528  1.1517
H   0.5480  2.9713  1.2933
H  -1.4568  1.5896  2.4490
C   0.6527  0.2730 -2.4414
C   1.8559  0.1288 -1.7000
C   1.8704 -1.1833 -1.1398
C   0.6823 -1.8499 -1.5549
C  -0.0713 -0.9510 -2.3481
H   0.3557  1.1451 -3.0127
H   2.6381  0.8712 -1.6035
H   2.6730 -1.6159 -0.5560
H   0.4035 -2.8674 -1.3087
H  -1.0196 -1.1668 -2.8226
C  -2.0745 -0.8163  0.1281
H -2.4706 -0.9391  1.1362
C  -2.5394  0.4671 -0.5326
H -2.2645 -1.7069 -0.4693
H -1.6720  1.2416 -0.6181
H -2.7800  0.3156 -1.5884
C  -3.6575  1.2432  0.1732
H -3.4241  1.4167  1.2271
H -4.5788  0.6559  0.1296
H -3.8432  2.2089 -0.3054
```

Cp2ZrCH(CH3)2+
268 -552.024786

```
Zr -1.2350 -0.1917 -4.4200
C  -0.6904  0.8078 -6.6882
C  -0.5993 -0.6114 -6.7998
C  -1.9137 -1.1465 -6.6552
C  -2.8034 -0.0672 -6.4213
C  -2.0441  1.1404 -6.4442
H   0.1298  1.5083 -6.7781
H   0.2950 -1.1763 -7.0329
H  -2.1859 -2.1910 -6.7320
H  -3.8772 -0.1416 -6.2928
H  -2.4419  2.1396 -6.3227
C  -1.9320 -1.8935 -2.6630
C  -1.3324 -2.6148 -3.7275
C   0.0454 -2.2488 -3.7867
C   0.2970 -1.3246 -2.7304
C  -0.9210 -1.0969 -2.0478
H  -2.9653 -1.9693 -2.3440
H  -1.8270 -3.3342 -4.3668
H   0.7841 -2.6612 -4.4627
H   1.2533 -0.8748 -2.4922
H  -1.0556 -0.4470 -1.1923
C  -0.0721  3.0044 -4.2158
C  -0.6544  1.8013 -3.4741
H   0.9557  2.8109 -4.5391
H  -0.6561  3.2777 -5.0996
H  -0.0396  3.8871 -3.5643
C  -2.1305  1.8912 -3.1218
H  -0.0630  1.5958 -2.5794
H  -2.7670  0.9969 -3.4746
H  -2.3469  1.8949 -2.0514
H  -2.6369  2.7285 -3.6072
```

Cp2ZrCH2CH(CH3)2+
292 -591.344352

```
Zr -0.0101 -0.0490 -0.0045
C  -0.1281 -0.0397  2.5368
C   1.2436 -0.1207  2.1524
C   1.6036  1.1204  1.5474
C   0.4522  1.9456  1.5225
C  -0.6149  1.2279  2.1394
H -0.6922 -0.8065  3.0521
H   1.9141 -0.9476  2.3536
H   2.5858  1.3879  1.1801
H   0.4005  2.9600  1.1436
H  -1.6131  1.6075  2.3075
C   0.4776 -0.0617 -2.4862
C   1.6807  0.3351 -1.8369
```

```
C  0.2131 -1.4160 -2.1360
H -0.1093  0.5479 -3.1627
H  2.1644  1.3004 -1.9267
H  3.0719 -0.8047 -0.5063
H  1.3439 -2.8440 -0.8406
H -0.6059 -2.0225 -2.4962
C -2.0755 -1.0074  0.0333
H -2.4805 -1.1583  1.0345
C -2.5871  0.2536 -0.6343
H -2.2044 -1.9055 -0.5698
H -1.6911  1.0172 -0.7393
C -3.0735  0.0682 -2.0817
C -3.6289  1.0407  0.1799
H -3.3498  1.1451  1.2295
H -4.5763  0.4940  0.1461
H -3.7988  2.0370 -0.2392
H -4.0094 -0.4987 -2.0636
H -3.2733  1.0312 -2.5614
H -2.3638 -0.4852 -2.6988
```

Cp2ZrC(CH3)3+
292 -591.333919

```
Zr -0.0007 -0.0815  0.0107
C  -0.0384  0.0448  2.5473
C   1.3273  0.0212  2.1332
C   1.6001  1.2488  1.4646
C   0.4017  2.0058  1.4241
C  -0.6076  1.2616  2.1046
H -0.5455 -0.7277  3.1102
H   2.0495 -0.7538  2.3604
H   2.5594  1.5580  1.0727
H   0.2866  2.9974  1.0024
H  -1.6253  1.5889  2.2723
C   0.9657  0.5023 -2.2780
C   2.0534  0.0805 -1.4720
C   1.8606 -1.2936 -1.1501
C   0.6687 -1.7307 -1.8026
C   0.1164 -0.6247 -2.4891
H   0.8330  1.4888 -2.7066
H   2.8934  0.6911 -1.1705
H   2.5421 -1.9158 -0.5825
H   0.2639 -2.7341 -1.7820
H  -0.7821 -0.6308 -3.0920
C  -2.8169 -1.2429  1.4010
C  -2.1470 -0.9888  0.0400
H -2.3773 -2.1087  1.9078
H -2.7658 -0.3908  2.0813
H -3.8814 -1.4750  1.2539
C  -2.5151  0.3495 -0.5758
C  -2.4449 -2.1903 -0.8732
H  -1.6324  1.0808 -0.7252
H  -2.9057  0.2797 -1.5937
H  -3.1857  0.9537  0.0397
H  -3.5280 -2.3769 -0.9010
H  -1.9816 -3.1066 -0.4917
H  -2.1172 -2.0500 -1.9048
```

Cp*2Zr(Cl)CH3
372 -1326.962160

```
Zr  0.0135  0.0859 -0.0114
C  -0.0342 -0.0341  2.6150
C   1.3414 -0.0506  2.2283
C   1.6587  1.2291  1.6792
C   0.4609  2.0086  1.6596
C  -0.5778  1.2333  2.2660
C   0.4230  0.8340 -2.4738
C   1.6970  0.8710 -1.8370
C   2.0625 -0.4752 -1.5058
C   1.0200 -1.3364 -1.9615
C  -0.0003 -0.5283 -2.5464
Cl -2.2624  0.9769 -0.5070
C  -0.7299 -2.0420  0.4171
H  0.0376 -2.7276  0.7993
H -1.5317 -1.9892  1.1601
H -1.1591 -2.4874 -0.4855
C   2.3237 -1.1445  2.5647
H   2.6287 -1.0855  3.6197
H   1.8939 -2.1406  2.4103
H   3.2333 -1.0764  1.9605
C   3.0532  1.7735  1.5038
H   3.0805  2.6452  0.8467
H   3.4407  2.0948  2.4819
H   3.7554  1.0318  1.1138
C   3.4157 -0.9592 -1.0465
H   3.9948 -0.1718 -0.5578
H   3.3391 -1.8007 -0.3493
H   4.0083 -1.3082 -1.9050
C   2.6002  2.0793 -1.8285
H   2.1066  2.9772 -1.4397
H   3.5042  1.9114 -1.2398
H   2.9192  2.3121 -2.8545
C   1.1172 -2.8369 -2.0193
H   1.5892 -3.2553 -1.1243
H   0.1374 -3.3093 -2.1256
H   1.7243 -3.1430 -2.8840
C  -0.2672  2.0175 -3.0994
H  -0.0718  2.9431 -2.5470
H   0.0887  2.1692 -4.1293
H  -1.3508  1.8806 -3.1337
C  -1.2389 -1.0301 -3.2392
H  -1.0397 -1.2176 -4.3042
H  -1.5967 -1.9685 -2.8031
```

```
H  0.4129  4.1201  2.1236
H  1.1264  3.7511  0.5512
H -0.6258  3.6562  0.7700
C  -1.9441  1.7364  2.6432
H  -1.9326  2.1262  3.6718
H  -2.2755  2.5407  1.9821
H  -2.7000  0.9473  2.5925
C  -0.7149 -1.0826  3.4518
H  -0.3531 -2.0895  3.2241
H  -0.5249 -0.8976  4.5191
H  -1.8001 -1.0791  3.3085
```

Cp*2Zr(Cl)CH2CH2CH3
420 -1405.581556

```
Zr  0.1441  0.0599  0.0194
C  -0.0328  0.0311  2.6732
C   1.3321  0.3167  2.3623
C   1.3804  1.6013  1.7391
C   0.0425  2.0843  1.6111
C  -0.8260  1.1200  2.2078
C   0.4795  0.9549 -2.4059
C   1.7041  1.2115 -1.7261
C   2.3131 -0.0510 -1.4216
C   1.4775 -1.0777 -1.9558
C   0.3353 -0.4591 -2.5421
Cl -2.2645  0.2952 -0.5968
C   0.9027 -3.1342  1.0661
C  -0.1298 -2.1904  0.4373
H   1.8756 -3.0368  0.5670
H   1.0820 -2.8442  2.1066
C   0.4847 -4.6135  1.0386
H  -1.0425 -2.1947  1.0515
H  -0.4466 -2.5937 -0.5349
H   1.2353 -5.2573  1.5115
H  -0.4653 -4.7604  1.5645
H   0.3435 -4.9630  0.0096
C   2.5513 -0.4416  2.8279
H   3.0857  0.1290  3.6023
H   2.2869 -1.4112  3.2578
H   3.2668 -0.6281  2.0175
C   2.6317  2.4333  1.6251
H   2.5067  3.2850  0.9568
H   2.8861  2.8385  2.6154
H   3.4963  1.8575  1.2882
C   3.7110 -0.2673 -0.8958
H   4.0660  0.5833 -0.3071
H   3.7797 -1.1602 -0.2642
H   4.4212 -0.4048 -1.7244
C   2.3767  2.5607 -1.6830
H   1.7010  3.3645 -1.3729
H   3.2415  2.5710 -1.0190
H   2.7392  2.8212 -2.6876
C   2.6515 -2.8246 -1.4367
H   1.0175 -3.2011 -1.9959
H   2.2478 -2.6801 -3.1500
C  -0.4162  2.0008 -3.0176
H  -0.3777  2.9453 -2.4645
H  -1.4593  1.6745 -3.0388
C  -0.7413 -1.1683 -3.3185
H  -0.4413 -1.2918 -4.3696
H  -0.9426 -2.1663 -2.9153
H  -1.6824 -0.6124 -3.2995
C  -0.3775  3.4450  1.1136
H  -0.4749  4.1562  1.9465
H   0.3504  3.8665  0.4130
H  -1.3455  3.4049  0.6036
C  -2.2906  1.3119  2.4929
H  -2.4241  1.8338  3.4530
H  -2.7843  1.9026  1.7171
H  -2.8188  0.3578  2.5555
C  -0.5594 -1.0810  3.5420
H   0.2282 -1.7815  3.8311
H  -0.9869 -0.6658  4.4661
H  -1.3514 -1.6593  3.0538
```

Cp*2Zr(Cl)CH(CH3)2
420 -1405.570336

```
Zr -0.0011 -0.0408 -0.0263
C   0.0192 -0.0277  2.6686
C   1.3810 -0.0022  2.2443
C   1.6163  1.2563  1.6068
C   0.3838  1.9723  1.5708
C  -0.6014  1.1789  2.2377
C   0.4109  0.8258 -2.4606
C   1.6836  0.8399 -1.8275
C   2.0504 -0.5169 -1.5469
C   1.0219 -1.3645 -2.0681
C   0.0022 -0.5338 -2.6162
Cl -2.2659  0.8854 -0.5346
C   0.0647 -3.2928  1.0055
C  -0.8494 -2.1625  0.5115
H   0.5909 -3.7754  0.1764
H   0.8259 -2.9548  1.7109
H  -0.5131 -4.0853  1.5068
H  -1.4264 -1.8153  1.3773
C  -1.9072 -2.7408 -0.4466
H  -2.6391 -1.9902 -0.7632
H  -2.4628 -3.5554  0.0462
H  -1.4687 -3.1763 -1.3474
C   2.4740 -0.9607  2.6523
H   3.1514 -0.4852  3.3767
```

```
H  3.0904 -1.2860  1.8066
C  2.9895  1.8478  1.4191
H  2.9771  2.7475  0.8018
H  3.3913  2.1367  2.4021
H  3.7035  1.1433  0.9833
C  3.4034 -1.0116 -1.0977
H  3.9597 -0.2509 -0.5438
H  3.3269 -1.8988 -0.4591
H  4.0187 -1.2944 -1.9646
C  2.5902  2.0442 -1.8103
H  2.1069  2.9382 -1.4024
H  3.5057  1.8655 -1.2452
H  2.8867  2.2875 -2.8408
C  1.1921 -2.8416 -2.3061
H  1.8048 -3.3172 -1.5358
H  0.2418 -3.3746 -2.3516
H  1.7015 -3.0010 -3.2677
C  0.2863  2.0259 -3.0449
H  0.0955  2.9339 -2.4632
H  0.0657  2.2126 -4.0704
H -1.3689  1.8822 -3.0809
C  -1.1974 -0.9744 -3.4124
H  -1.0163 -0.8209 -4.4875
H  -1.4221 -2.0337 -3.2623
H  -2.0925 -0.4020 -3.1411
C   0.1761  3.3864  1.0884
H   0.1682  4.0917  1.9320
H   0.9717  3.7058  0.4076
H  -0.7780  3.4964  0.5616
C  -1.9839  1.6316  2.6222
H  -1.9743  2.0584  3.6362
H  -2.3633  2.3948  1.9389
H  -2.7033  0.8066  2.6152
C  -0.6148 -1.0311  3.5938
H  -0.1102 -2.0028  3.5615
H  -0.5698 -0.6661  4.6326
H  -1.6738 -1.1990  3.3586
```

Cp*2Zr(Cl)CH2CH(CH3)2
444 -1444.890386

```
Zr  0.0500 -0.0431 -0.0299
C   0.0337 -0.0246  2.6388
C   1.4033  0.0173  2.2355
C   1.6288  1.2712  1.5877
C   0.3860  1.9788  1.5446
C  -0.5903  1.1809  2.2137
C   0.3159  0.9197 -2.4420
C   1.6232  0.9396 -1.8796
C   2.0430 -0.4177 -1.6817
C   1.0084 -1.2672 -2.1789
C  -0.0686 -0.4452 -2.6187
Cl -2.3255  0.6431 -0.4476
C   0.0482 -3.3865  1.2385
C  -0.5590 -2.2345  0.4081
C   1.3613 -3.9589  0.6821
H   1.7932 -4.6899  1.3769
H   2.1058 -3.1748  0.5151
H   1.1972 -4.4770 -0.2672
H   0.2749 -3.0028  2.2379
C  -0.9676 -4.5311  1.4252
H  -1.5059 -1.9438  0.8983
H  -0.8731 -2.6358 -0.5668
H  -0.5573 -5.3384  2.0454
H  -1.8866 -4.1725  1.9014
H  -1.2450 -4.9634  0.4557
C   2.4940 -0.9434  2.6380
H   2.9843 -0.6071  3.5638
H   2.1094 -1.9507  2.8180
H   3.2731 -1.0208  1.8720
C   2.9955  1.8733  1.3810
H   2.9658  2.7665  0.7552
H   3.4074  2.1748  2.3656
H   3.7105  1.1720  0.9405
C   3.4339 -0.8761 -1.3150
H   3.9501 -0.1589 -0.6701
H   3.4225 -1.8401 -0.7951
H   4.0525 -1.0015 -2.2158
C   2.5138  2.1563 -1.8653
H   2.0225  3.0414 -1.4479
H   3.4370  1.9863 -1.3089
H   2.7994  2.4097 -2.8967
C   1.1370 -2.7327 -2.4911
H   1.9781 -3.1926 -1.9688
H   0.2360 -3.3001 -2.2375
H   1.3089 -2.8640 -3.5694
C  -0.4419  2.1274 -2.9270
H  -0.2318  3.0133 -2.3180
H  -0.1598  2.3678 -3.9629
H  -1.5217  1.9603 -2.9021
C  -1.3071 -0.9366 -3.3188
H  -1.1141 -1.0721 -4.3934
H  -1.6427 -1.9010 -2.9225
H  -2.1362 -0.2329 -3.2099
C   0.1645  3.3909  1.0629
H   0.1578  4.0959  1.9066
H   0.9515  3.7166  0.3758
H  -0.7952  3.4939  0.5445
C  -1.9759  1.6142  2.6045
H  -1.9642  2.0375  3.6203
H  -2.3702  2.3750  1.9268
H  -2.6822  0.7790  2.5981
C  -0.6188 -1.0087  3.5777
H   0.0886 -1.7629  3.9311
```

```
H -1.4693 -1.5331  3.1274
```

Cp*2Zr(Cl)CH(CH3)3
444 -1444.866378

```
Zr -0.0284 -0.0173  0.0259
C   0.1445 -0.0323  2.7423
C   1.4745  0.0169  2.2208
C   1.6546  1.2913  1.6034
C   0.4040  1.9764  1.6323
C  -0.5283  1.1592  2.3504
C   0.4433  0.8183 -2.4393
C   1.6955  0.8558 -1.7706
C   2.0691 -0.4921 -1.4626
C   1.0703 -1.3593 -2.0124
C   0.0589 -0.5465 -2.6014
Cl -2.1718  1.1247 -0.5280
C  -1.1905 -2.1022  0.4617
C  -0.2866 -3.2124  1.0298
H   0.4808 -3.5257  0.3151
H   0.2309 -2.9236  1.9483
H  -0.8795 -4.1134  1.2680
C  -2.3631 -1.8496  1.4376
H  -3.0731 -1.1258  1.0268
H  -2.0612 -1.4979  2.4195
H  -2.9160 -2.7928  1.5952
C  -1.8823 -2.6686 -0.7947
H  -2.5481 -1.9371 -1.2618
H  -2.5082 -3.5328 -0.5096
H  -1.1847 -3.0275 -1.5486
C   2.5730 -0.9504  2.5856
H   2.9678 -0.7302  3.5893
H   2.2170 -1.9861  2.6007
H   3.4143 -0.8978  1.8891
C   2.9994  1.9363  1.3896
H   2.9415  2.8354  0.7753
H   3.3985  2.2410  2.3687
H   3.7371  1.2635  0.9457
C   3.4237 -0.9767 -1.0081
H   3.9816 -0.2081 -0.4680
H   3.3508 -1.8553 -0.3579
H   4.0352 -1.2700 -1.8747
C   2.5881  2.0711 -1.7765
H   2.1082  2.9607 -1.3549
H   3.5232  1.9023 -1.2420
H   2.8483  2.3165 -2.8163
C   1.3102 -2.8301 -2.2465
H   1.6492 -3.3568 -1.3492
H   0.4233 -3.3468 -2.6181
H   2.0978 -2.9521 -3.0051
C  -0.2390  1.9979 -3.0779
H  -0.0615  2.9232 -2.5204
H   0.1381  2.1495 -4.1008
H  -1.3208  1.8542 -3.1338
C  -1.0940 -0.9713 -3.4738
H  -0.9370 -0.6088 -4.4992
H  -1.2020 -2.0564 -3.5199
H  -2.0443 -0.5535 -3.1233
C   0.1482  3.3935  1.1833
H   0.2133  4.0900  2.0318
H   0.8777  3.7235  0.4363
H  -0.8482  3.5014  0.7435
C  -1.8987  1.5961  2.7957
H  -1.8382  2.1334  3.7535
H  -2.3609  2.2640  2.0643
H  -2.5761  0.7481  2.9295
C  -0.2736 -0.9539  3.8621
H  -0.2014 -2.0169  3.6184
H   0.3828 -0.7773  4.7269
H  -1.2967 -0.7546  4.1902
```

D. CpFe compounds.

CpFe(CO)2CH3
196 -583.578213

```
Fe -0.0784  0.0051  0.3744
C   0.0356 -0.0767  2.5311
C   1.3555  0.0065  1.9902
C   1.5742 -1.1265  1.1624
C   0.3931 -1.9283  1.1934
C  -0.5464 -1.2834  2.0449
H   2.0591  0.8109  2.1610
H   2.4688 -1.3334  0.5916
H   0.2363 -2.8535  0.6566
H  -1.5472 -1.6342  2.2618
H  -0.4298  0.6365  3.1973
C  -1.7564  0.1082 -0.1439
O  -2.8573  0.1503 -0.4879
C   0.3226  1.6418 -0.1300
O   0.6170  2.7039 -0.4729
C   0.3743 -0.5608 -1.5389
H   0.0683 -1.6027 -1.6699
H   1.4560 -0.4821 -1.6817
H  -0.1178  0.0399 -2.3087
```

CpFe(CO)2CH2CH2CH3
244 -662.206390

```
Fe -0.0839  0.0023  0.3430
C   0.0308 -0.1071  2.5037
C   1.3486 -0.0236  1.9619
C   1.5622 -1.1483  1.1192
C   0.3771 -1.9438  1.1427
C  -0.5593 -1.3043  2.0007
```

```
H  2.4579 -1.3556  0.5500
H  0.2141 -2.8620  0.5956
H -1.5613 -1.6534  2.2140
H -0.4305  0.6011  3.1777
C  -1.7759  0.1682 -0.1109
O  -2.8932  0.2532 -0.3909
C   0.3663  1.6285 -0.1556
O   0.6884  2.6883 -0.4823
C   0.3316 -0.6142 -1.5842
H   1.4256 -0.5900 -1.6573
H   0.0224 -1.6657 -1.6094
C  -0.2683  0.1152 -2.7877
H  -1.3646  0.0880 -2.7437
H   0.0104  1.1768 -2.7722
C   0.1834 -0.4917 -4.1256
H   1.2733 -0.4430 -4.2322
H  -0.1083 -1.5460 -4.1979
H  -0.2604  0.0376 -4.9768
```

CpFe(CO)2CH(CH3)2
244 -662.203984

```
Fe -0.1177 -0.0380  0.3224
C   0.5604  0.3098  2.3427
C   1.6898  0.0849  1.4842
C   1.5777 -1.2309  0.9607
C   0.3794 -1.8102  1.4501
C  -0.2438 -0.8514  2.3220
H   2.4912  0.7845  1.2901
H   2.2574 -1.6918  0.2578
H   0.0102 -2.8017  1.2255
H  -1.1794 -0.9866  2.8483
H   0.3497  1.2192  2.8894
C  -1.7617 -0.5050 -0.0968
O  -2.8455 -0.8359 -0.3210
C  -0.3073  1.6453 -0.1391
O  -0.4114  2.7526 -0.4521
C   0.4905 -0.3808 -1.6495
H   0.6366 -1.4680 -1.6385
C   1.8264  0.3008 -1.9662
H   1.7304  1.3933 -1.9743
H   2.6196  0.0495 -1.2562
H   2.1814  0.0070 -2.9662
C  -0.5222 -0.0532 -2.7513
H  -0.1050 -0.2934 -3.7409
H  -1.4544 -0.6167 -2.6505
H  -0.7795  1.0130 -2.7696
```

CpFe(CO){P(CH3)3}CH3
246 -931.346817

```
Fe -0.0375 -0.0208  0.3012
C  -0.1268 -0.1564  2.4683
C   1.2445 -0.2030  2.0630
C   1.4279 -1.3299  1.2250
C   0.1711 -1.9968  1.1010
C  -0.7783 -1.2767  1.8791
H   2.0150  0.5009  2.3521
H   2.3494 -1.6179  0.7377
H  -0.0244 -2.8854  0.5172
H  -1.8268 -1.5243  1.9829
H  -0.5777  0.5741  3.1260
O  -2.6475  0.3508 -0.9038
C  -1.6012  0.2140 -0.4145
P   0.6024  2.0623 -0.0936
C   0.3667  3.2701  1.2911
H  -0.6936  3.3063  1.5611
H   0.9281  2.9423  2.1717
H   0.6999  4.2771  1.0142
C   2.3897  2.3017 -0.5085
H   3.0113  1.9348  0.3147
H   2.6308  1.7151 -1.3998
H   2.6293  3.3550 -0.6936
C  -0.2316  2.9373 -1.4894
H   0.1597  3.9517 -1.6221
H  -0.0820  2.3711 -2.4133
H  -1.3077  2.9901 -1.2977
C   0.6611 -0.5322 -1.5451
H   1.7586 -0.5259 -1.5486
H   0.3317 -1.5524 -1.7720
H   0.3235  0.1008 -2.3746
```

CpFe(CO){P(CH3)3}CH2CH2CH3
294 -1009.971890

```
Fe  0.1515  0.9047  0.0801
C  -1.6020  2.1951 -0.0001
C  -0.5990  2.7049 -0.8946
C   0.5438  3.0307 -0.1264
C   0.2796  2.7075  1.2352
C  -1.0599  2.2095  1.3064
H  -0.7059  2.8424 -1.9630
H   1.4817  3.4020 -0.5167
H   0.9616  2.8295  2.0654
H  -1.5613  1.8681  2.2027
H  -2.5975  1.8721 -0.2715
O   0.2358 -1.2093  2.0650
C   0.2037 -0.3729  1.2572
P  -0.3919 -0.4403 -1.6148
C  -2.1067 -0.2408 -2.2965
H  -2.8414 -0.4201 -1.5053
H  -2.2495  0.7772 -2.6718
H  -2.2881 -0.9457 -3.1160
C   0.6067 -0.2978 -3.1696
H   0.5708  0.7351 -3.5310
H   1.6515 -0.5449 -2.9642
```

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H 0.2267 -0.9643 -3.9522
C -0.3793 -2.2660 -1.3105
H -0.6492 -2.8226 -2.2150
H 0.6096 -2.5865 -0.9735
H -1.0970 -2.5018 -0.5182
C 2.1593 0.6534 -0.2879
H 2.3481 1.1023 -1.2751
H 2.6435 1.3105 0.4472
C 2.8659 -0.7044 -0.2239
H 2.7003 -1.1719 0.7555
H 2.4448 -1.4034 -0.9602
C 4.3795 -0.6063 -0.4736
H 4.5889 -0.1808 -1.4627
H 4.8551 0.0450 0.2690
H 4.8672 -1.5874 -0.4203

CpFe(CO){P(CH3)3}CH(CH3)3
294 -1009.963501
Fe 0.1743 0.9205 0.0399
C -1.5199 2.2417 0.4808
C -1.0797 2.5117 -0.8370
C 0.2785 2.9461 -0.7917
C 0.6673 2.9638 0.5755
C -0.4228 2.5173 1.3631
H -1.6731 2.4092 -1.7354
H 0.8895 3.2331 -1.6368
H 1.6458 3.2303 0.9466
H -0.4312 2.4147 2.4398
H -2.5027 1.8944 0.7699
O -0.2693 -1.2824 1.8704
C -0.0916 -0.3957 1.1382
P -0.3017 -0.3893 -1.7285
C -2.1199 -0.4718 -2.1081
H -2.6531 -0.8340 -1.2233
H -2.5168 0.5138 -2.3622
H -2.3152 -1.1537 -2.9439
C 0.3854 0.0950 -3.3795
H 0.0708 1.1163 -3.6172
H 1.4785 0.0790 -3.3446
H 0.0412 -0.5767 -4.1745
C 0.0389 -2.2083 -1.6804
H -0.4073 -2.7006 -2.5516
H 1.1108 -2.4072 -1.6672
H -0.3982 -2.6318 -0.7707
C 2.2216 0.5507 0.1593
H 2.6263 1.4102 -0.3933
C 2.8218 -0.7049 -0.4774
H 2.4348 -1.6227 -0.0173
H 2.6403 -0.7642 -1.5560
C 2.7260 0.6346 1.6098
H 3.8269 0.6586 1.6493
H 2.3616 1.5179 2.1424
H 2.4073 -0.2398 2.1909
H 3.9154 -0.7275 -0.3454

E. Palladium complexes
{Pd}R, with [Pd] = {(CH3)2NCS2}Pd{P(CH3)3}

[Pd]CH3
242 -1596.898737
(368 -1597.066840)
Pd 0.0391 0.0033 0.0220
P -0.0091 0.0531 2.3079
C -0.8076 -1.3957 3.1287
H -0.8082 -1.2887 4.2197
H -1.8376 -1.4960 2.7748
H -0.2650 -2.3063 2.8569
C 1.6475 0.1154 3.1212
H 2.2307 -0.7613 2.8232
H 2.1838 1.0070 2.7823
H 1.5599 0.1383 4.2136
C -0.8836 1.4947 3.0611
H -0.3895 2.4188 2.7459
H -1.9170 1.5236 2.7043
H -0.8797 1.4391 4.1560
S 2.4893 0.0380 -0.4543
S 0.2871 -0.0464 -2.3970
C 1.9989 0.0033 -2.1194
N 2.8824 0.0127 -3.1375
C 2.4360 -0.1258 -4.5241
H 2.2691 -1.1793 -4.7838
H 1.5043 0.4214 -4.6732
H 3.2058 0.2861 -5.1817
C 4.3242 -0.0727 -2.9102
H 4.5668 0.3223 -1.9245
H 4.6702 -1.1134 -2.9697
H 4.8400 0.5167 -3.6741
C -2.0351 -0.0450 -0.0420
H -2.5540 -0.0395 0.9213
H -2.3465 0.8322 -0.6182
H -2.3053 -0.9566 -0.5846

[Pd]CH2CH2CH3
290 -1675.528195
(440 -1675.713585)
Pd 0.0073 0.0013 -0.0406
P 0.0260 -0.0264 2.2502
C 1.6731 -0.2080 3.0665
H 1.5771 -0.2371 4.1581
H 2.1545 -1.1284 2.7236
H 2.3114 0.6351 2.7847
H -1.6832 1.6473 2.7193
H -0.6291 1.4175 4.1436
C -0.9707 -1.3701 3.0351
H -2.0152 -1.2713 2.7240
H -0.6063 -2.3442 2.6957
H -0.9144 -1.3253 4.1291
S -1.2268 2.1315 -0.5106
S -0.1502 0.2135 -2.4631
C -1.0052 1.6974 -2.1770
N -1.4603 2.4505 -3.1970
C -1.2284 2.0639 -4.5891
H -0.2271 2.3663 -4.9209
H -1.3214 0.9827 -4.7003
H -1.9767 2.5577 -5.2148
C -2.0955 3.7522 -3.0031
H -2.1778 3.9684 -1.9395
H -1.4961 4.5347 -3.4852
H -3.0962 3.7482 -3.4513
C 1.0566 -1.8018 -0.0896
H 1.0063 -2.3468 0.8621
H 0.5154 -2.4012 -0.8322
C 2.5144 -1.6008 -0.5040
C 3.2835 -2.9275 -0.6367
H 3.0296 -0.9627 0.2269
H 2.5579 -1.0613 -1.4577
H 4.3261 -2.7596 -0.9317
H 2.8213 -3.5750 -1.3905
H 3.2886 -3.4787 0.3115

[Pd]CH(CH3)2
290 -1675.526954
(440 -1675.712905)
Pd 0.0208 -0.0107 -0.0249
P -0.0091 -0.0169 2.2676
C 1.6378 -0.0021 3.1062
H 1.5336 -0.0238 4.1973
H 2.2236 -0.8683 2.7845
H 2.1806 0.9024 2.8151
C -0.8595 1.4337 3.0292
H -0.3647 2.3542 2.7048
H -1.8960 1.4688 2.6802
H -0.8461 1.3800 4.1239
C -0.8650 -1.4467 3.0674
H -1.9130 -1.4598 2.7525
H -0.4013 -2.3832 2.7436
H -0.8186 -1.3821 4.1607
S -1.1842 2.1550 -0.5026
S -0.0973 0.2436 -2.4561
C -0.9426 1.7314 -2.1677
N -1.3752 2.4930 -3.1915
C -1.1158 2.1097 -4.5803
H -0.0857 2.3510 -4.8709
H -1.2718 1.0376 -4.7117
H -1.8076 2.6576 -5.2253
C -2.0043 3.7983 -3.0019
H -2.1378 3.9919 -1.9391
H -1.3740 4.5850 -3.4354
H -2.9808 3.8146 -3.5000
C 1.0431 -1.8502 -0.0287
H 1.2297 -2.1621 1.0071
C 0.1697 -2.9112 -0.6967
C 2.3934 -1.6767 -0.7222
H 2.9505 -2.6283 -0.7321
H 3.0204 -0.9327 -0.2189
H 2.2767 -1.3572 -1.7631
H -0.0630 -2.6489 -1.7340
H -0.7816 -3.0498 -0.1717
H 0.6852 -3.8860 -0.7126

[Pd]CH2CH(CH3)2
314 -1714.842231
(476 -1715.035572)
Pd 0.0393 0.0200 -0.0836
P 0.0831 -0.0083 2.2148
C 1.6979 -0.2055 3.0913
H 1.5580 -0.1966 4.1785
H 2.1665 -1.1494 2.7994
H 2.3705 0.6104 2.8098
C -0.6037 1.5142 3.0028
H -0.0024 2.3794 2.7077
H -1.6253 1.6774 2.6468
H -0.6092 1.4324 4.0960
C -0.9416 -1.3478 2.9708
H -1.9765 -1.2456 2.6302
H -0.5706 -2.3230 2.6412
H -0.9153 -1.3037 4.0660
S -1.4646 1.9929 -0.4655
S -0.3016 0.2102 -2.4919
C -1.3139 1.5753 -2.1442
N -1.9321 2.2580 -3.1271
C -1.7540 1.8917 -4.5326
H -0.8213 2.3080 -4.9337
H -1.7258 0.8062 -4.6383
H -2.5976 2.2890 -5.1033
C -2.7096 3.4716 -2.8853
H -2.7459 3.6804 -1.8176
H -2.2462 4.3208 -3.4032
H -3.7300 3.3412 -3.2646
C 1.2696 -1.6741 -0.1680
H 1.0397 -2.3383 0.6754
H 0.9469 -2.1932 -1.0791
C 2.7800 -1.4008 -0.2204
C 3.2002 -0.5977 -1.4598
H 4.6460 -2.5538 -0.1515
H 3.3268 -3.3633 -1.0141
H 3.3142 -3.2961 0.7537
H 2.7015 0.3752 -1.4931
H 2.9331 -1.1341 -2.3793
H 4.2843 -0.4324 -1.4743

[Pd]C(CH3)3
314 -1714.834002
(476 -1715.027208)
Pd 0.1031 -0.0357 0.0157
P -0.1739 0.0292 2.3339
C 1.2923 0.1845 3.4540
H 0.9769 0.2971 4.4979
H 1.9386 -0.6911 3.3667
H 1.8690 1.0671 3.1592
C -1.1536 1.5093 2.8519
H -0.6245 2.4208 2.5588
H -2.1224 1.5053 2.3446
H -1.3095 1.5157 3.9370
C -1.1632 -1.3269 3.1178
H -2.1417 -1.3745 2.6293
H -0.6716 -2.2942 2.9873
H -1.3067 -1.1405 4.1886
S -1.0556 2.2014 -0.4129
S -0.0645 0.2983 -2.4054
C -0.8980 1.7832 -2.0850
N -1.3797 2.5438 -3.0872
C -1.1890 2.1575 -4.4863
H -0.1715 2.3888 -4.8251
H -1.3614 1.0868 -4.6092
H -1.9050 2.7115 -5.0986
C -1.9959 3.8506 -2.8677
H -2.0859 4.0395 -1.7994
H -1.3813 4.6377 -3.3229
H -2.9918 3.8719 -3.3256
C 1.0479 -1.9485 -0.1321
C 1.8450 -2.3674 1.1057
C -0.0804 -2.9474 -0.4020
C 2.0240 -1.9075 -1.3146
H 2.5555 -2.8715 -1.3879
H 2.7805 -1.1249 -1.1946
H 1.5235 -1.7461 -2.2725
H -0.6574 -2.6756 -1.2913
H -0.7767 -3.0188 0.4407
H 0.3334 -3.9573 -0.5706
H 1.2206 -2.4899 1.9950
H 2.6424 -1.6534 1.3366
H 2.3277 -3.3428 0.9272

[Pd]CH2CH2CN
289 -1728.451103
(441 -1728.658116)
Pd -0.0019 -0.0106 -0.0442
P 0.0230 -0.0320 2.2575
C 1.6664 -0.2613 3.0682
H 1.5704 -0.2804 4.1599
H 2.1186 -1.2002 2.7356
H 2.3311 0.5599 2.7827
C -0.6118 1.5059 3.0549
H 0.0006 2.3568 2.7418
H -1.6387 1.6891 2.7241
H -0.5923 1.4279 4.1480
C -1.0098 -1.3547 3.0269
H -2.0501 -1.2285 2.7118
H -0.6675 -2.3355 2.6837
H -0.9572 -1.3176 4.1212
S -1.2329 2.0973 -0.5077
S -0.1599 0.1839 -2.4586
C -1.0039 1.6759 -2.1774
N -1.4420 2.4345 -3.1964
C -1.2068 2.0449 -4.5885
H -0.1964 2.3260 -4.9102
H -1.3239 0.9663 -4.7032
H -1.9389 2.5562 -5.2187
C -2.0654 3.7430 -3.0037
H -2.1487 3.9610 -1.9405
H -1.4556 4.5179 -3.4844
H -3.0643 3.7482 -3.4549
C 1.0593 -1.8047 -0.0977
H 1.1035 -2.3228 0.8654
H 0.5181 -2.4524 -0.7945
C 2.4911 -1.5453 -0.6092
C 3.3075 -2.7662 -0.6352
H 3.0061 -0.8120 0.0232
H 2.4680 -1.1175 -1.6177
N 3.9317 -3.7458 -0.6313

[Pd]CH(CN)(CH3)
289 -1728.462455
(441 -1728.667905)
Pd -0.0955 -0.0973 -0.1570
P 0.1577 0.1345 2.1530
C 1.8224 0.7734 2.6136
H 1.8984 0.9360 3.6951
H 2.5756 0.0450 2.2984
H 2.0042 1.7175 2.0910
C -1.0029 1.3674 2.8894
H -0.8911 2.3309 2.3841
H -2.0346 1.0300 2.7519
H -0.8047 1.4982 3.9594
C -0.0598 -1.3263 2.3596
H 0.6900 -2.0829 3.0160
H 0.0604 -1.0308 4.3081
S -0.8076 2.2339 -0.5590
S -0.4136 0.1378 -2.5538
C -0.8580 1.7822 -2.2341
N -1.2134 2.6248 -3.2173
C -1.2075 2.1929 -4.6169
H -0.1894 2.1967 -5.0245
H -1.6147 1.1837 -4.7015
H -1.8286 2.8823 -5.1938
C -1.5152 4.0368 -2.9859
H -1.4709 4.2559 -1.9204
H -0.7877 4.6656 -3.5133
H -2.5194 4.2659 -3.3606
C 0.4690 -2.1451 -0.1395
H -0.2926 -2.6298 0.4824
C 0.5201 -2.8039 -1.5250
C 1.7365 -2.2324 0.5500
N 2.7474 -2.2748 1.1340
H 1.2508 -2.3128 -2.1735
H -0.4586 -2.7455 -2.0081
H 0.7996 -3.8632 -1.4487

[Pd]CH2CH2CF3
329 -1973.279598
(485 -1973.547756)
Pd 0.0208 0.0331 -0.0185
P -0.0092 0.0207 2.2831
C 1.6238 0.0279 3.1431
H 1.4968 -0.0055 4.2313
H 2.2183 -0.8341 2.8270
H 2.1698 0.9380 2.8757
C -0.8775 1.4565 3.0525
H -0.3818 2.3850 2.7536
H -1.9095 1.4936 2.6904
H -0.8804 1.3832 4.1460
C -0.8720 -1.4295 3.0325
H -1.9099 -1.4486 2.6866
H -0.3881 -2.3555 2.7085
H -0.8575 -1.3801 4.1275
S -1.4694 1.9628 -0.4957
S -0.1381 0.2078 -2.4371
C -1.1926 1.5605 -2.1623
N -1.7504 2.2351 -3.1825
C -1.4754 1.8717 -4.5741
H -0.5201 2.2939 -4.9094
H -1.4356 0.7866 -4.6797
H -2.2804 2.2661 -5.1993
C -2.5677 3.4324 -2.9919
H -2.6674 3.6485 -1.9297
H -2.0950 4.2872 -3.4909
H -3.5625 3.2761 -3.4249
C 1.2962 -1.6239 -0.0355
C H 1.3617 -2.1181 0.9383
H 0.8370 -2.3285 -0.7356
C 2.6904 -1.2138 -0.5120
C 3.7013 -2.3433 -0.4958
H 3.1191 -0.4236 0.1136
H 2.6612 -0.8297 -1.5365
F 3.3312 -3.4008 -1.2622
F 3.9078 -2.8332 0.7622
F 4.9206 -1.9415 -0.9528

[Pd]CH(CH3)(CF3)
329 -1973.278890
(485 -1973.548718)
Pd -0.0154 0.0187 0.1358
P -0.1843 0.0724 2.4505
C 1.4231 0.4648 3.2640
H 1.3052 0.5743 4.3484
H 2.1371 -0.3357 3.0526
H 1.8175 1.3958 2.8460
C -1.2985 1.4182 3.0495
H -0.9840 2.3750 2.6234
H -2.3220 1.2214 2.7156
H -1.2828 1.4857 4.1434
C -0.7944 -1.3880 3.3981
H -1.8020 -1.6537 3.0627
H -0.1343 -2.2430 3.2319
H -0.8257 -1.1624 4.4700
S 0.1940 2.4717 -0.1328
S 0.2044 0.4538 -2.2483
C 0.2668 2.1338 -1.8360
N 0.3570 3.0926 -2.7727
C 0.4234 2.7507 -4.1954
H 1.4317 2.4225 -4.4749
H -0.2815 1.9488 -4.4232
H 0.1602 3.6382 -4.7759
C 0.5018 4.5115 -2.4508
H 0.4740 4.6523 -1.3717
H 1.4576 4.8852 -2.8376
H -0.3136 5.0815 -2.9110
C -0.2146 -2.0818 0.0254
H -0.8113 -2.4030 0.8839
C -0.9151 -2.5370 -1.2581
C 1.1164 -2.7590 0.1918
H -0.3254 -2.3063 -2.1495
H -1.8785 -2.0305 -1.3579
H -1.1007 -3.6193 -1.2511
F 1.7325 -2.4481 1.3794
F 2.0117 -2.4733 -0.7867
F 1.0146 -4.1322 0.2091

F. diimino-Pd complexes
[Pd](L)(R), where [Pd] = (diimine)Pd.

F1. Free ligands (L)

C2H4 36 -78.585789
C 0.0000 0.0000 0.6659
C 0.0000 0.0000 -0.6659
H 0.0000 0.9240 1.2396
H 0.0000 -0.9240 1.2396
H 0.0000 0.9240 -1.2396
H 0.0000 -0.9240 -1.2396

(CH3)2O 54 -155.022459
O -0.6354 -2.2311 -0.1119
C -1.4930 -2.7537 -1.1000
H -2.3894 -3.2218 -0.6595
H -1.8057 -1.9201 -1.7349
H -0.9865 -3.5078 -1.7253
C -0.1772 -3.2203 0.7806
H 0.3948 -4.0080 0.2620
H 0.4769 -2.7280 1.5055
H -1.0093 -3.7021 1.3207

CH3CN 48 -132.751634
N 0.0000 0.0000 -1.3273
C 0.0000 0.0000 -0.1672
C 0.0000 0.0000 1.2944
H -1.0267 0.0000 1.6737
H 0.5134 0.8892 1.6737
H 0.5134 -0.8892 1.6737

(CH3)2S 66 -478.039013
S 0.0115 0.0301 -0.0242
C -0.1386 0.0076 1.7948
H 0.7083 -0.5095 2.2557
H -0.1401 1.0487 2.1284
H -1.0750 -0.4633 2.1090
C 0.0052 -1.7674 -0.3424
H -0.9295 -2.2256 -0.0055
H 0.0941 -1.9015 -1.4237
H 0.8539 -2.2585 0.1433

F2. Compound from ref. 13 with X-Ray structure

{ArNCHCHNAr}PdCl(CH3)
424 -1748.650143
Pd -0.0621 0.0270 -0.0290
N 0.0201 -0.0208 2.2177
N 1.9942 -0.0040 0.3927
C 1.2351 0.0079 2.6438
C 2.3063 -0.0177 1.6499
C -1.0760 0.0524 3.1455
C -1.8385 -1.1200 3.3600
C -2.9122 -1.0485 4.2592
C -3.2423 0.1523 4.8941
C -2.5062 1.3082 4.6266
C -1.4114 1.2896 3.7458
H -3.5032 -1.9374 4.4525
H -4.0832 0.1906 5.5797
H -2.7933 2.2454 5.0926
C 3.0729 -0.0449 -0.5754
C 3.5777 1.1757 -1.0817
C 4.6278 1.1130 -2.0122
C 5.1399 -0.1136 -2.4428
C 4.5947 -1.3051 -1.9591
C 3.5456 -1.2995 -1.0245
H 5.0414 2.0349 -2.4075
H 5.9517 -0.1404 -3.1630
H 4.9799 -2.2549 -2.3161
C 0.1097 0.1243 -2.0539
H 1.1700 0.1395 -2.3150
H -0.3897 -0.7526 -2.4722
H -0.3954 1.0302 -2.3962
H 3.3482 -0.0492 1.9703
H 1.4828 0.0607 3.7066
C -0.7586 -3.4026 3.6188
C -1.4898 -2.4329 2.6582
H 0.1562 -2.9527 4.0247
H -1.4021 -3.6717 4.4656
H -0.4834 -4.3259 3.0944
C -2.7269 -3.1024 2.0214
H -0.8031 -2.1942 1.8371
H -3.2130 -2.4164 1.3212
H -2.4222 -4.0000 1.4696
H -3.4586 -3.4115 2.7778
C -1.6441 3.5264 2.5862
C -0.7013 2.5999 3.3938
H -2.0056 3.0207 1.6846
H -2.5148 3.8190 3.1850
H -1.1152 4.4398 2.2861
C -0.1422 3.3192 4.6423
H 0.1480 2.3710 2.7417
H 0.5540 2.6774 5.1959
H 0.3909 4.2313 4.3479
H -0.9452 3.6110 5.3290
C 2.3374 -3.4149 -1.7426
C 2.9328 -2.6211 -0.5550
H 1.5879 -2.8186 -2.2733
H 3.1142 -3.7049 -2.4602
H 1.8543 -4.3305 -1.3812
H 2.1017 -2.3910 0.1201
H 4.3467 -2.9342 1.0987
H 3.4835 -4.4006 0.5867
H 4.8060 -3.7552 -0.4021
C 4.0130 3.2927 0.2549
C 3.0123 2.5291 -0.6456
H 4.2737 2.7109 1.1474
H 4.9425 3.5064 -0.2869
H 3.5831 4.2472 0.5812
C 2.5876 3.3918 -1.8564
H 2.1070 2.3416 -0.0570
H 1.8665 2.8573 -2.4832
H 2.1182 4.3199 -1.5098
H 3.4469 3.6656 -2.4801
Cl -2.3799 0.0830 -0.3139

F3. "model" compounds, (diimine) = HNCHCHNH

[Pd]CH3+
124 -354.519009
Pd -0.0187 -0.0074 -0.0169
N 0.0530 -0.0335 2.2287
N 1.9862 0.0496 0.4038
C 1.2578 -0.0036 2.6614
C 2.3342 0.0446 1.6398
H -0.6627 -0.0671 2.9574
H 2.7373 0.0835 -0.2864
C 0.1764 0.0186 -2.0075
H 0.6386 0.9501 -2.3414
H 0.7266 -0.8560 -2.3605
H -0.8852 -0.0307 -2.2987
H 3.3803 0.0743 1.9437
H 1.5276 -0.0118 3.7176

[Pd]CH2CH2CH3+
172 -433.177733
Pd 0.0009 0.0121 0.0125
N 0.0022 0.0216 2.2293
N 2.0320 -0.0182 0.5399
C 1.1756 0.0182 2.7414
C 2.3157 -0.0134 1.7905
H -0.7614 0.0459 2.9067
H 2.8314 -0.0410 -0.0939
C -0.0640 0.0615 -2.0255
H 0.3785 0.9884 -2.3897
C -1.5198 0.0399 -1.7626
C -2.3128 -1.1842 -2.2436
H -1.6800 0.0541 -0.5740
H 3.3396 -0.0307 2.1639
H 1.3716 0.0376 3.8139
H 0.3820 -0.8379 -2.4523
H -1.8074 -2.1126 -1.9653
H -2.4016 -1.1577 -3.3336
H -3.3202 -1.1932 -1.8215
H -2.0085 0.9901 -2.0146

[Pd]CH(CH3)2+
172 -433.180800
Pd -0.0261 0.0154 -0.0064
N 0.0657 -0.0091 2.2298
N 2.0341 0.0406 0.4593
C 1.2585 0.0243 2.6934
C 2.3621 0.0364 1.6992
H -0.6659 -0.0071 2.9433
H 2.8177 0.0503 -0.1956
C -0.1903 0.0972 -2.0568
H 0.2001 1.0702 -2.3628
C -1.6250 0.0849 -1.6888
H -2.1744 -0.8051 -2.0017
H -1.7570 0.0250 -0.5028
H 3.3982 0.0407 2.0369
H 1.4975 0.0493 3.7570
C 0.4039 -1.0708 -2.8055
H 1.4970 -1.0494 -2.7808
H 0.0594 -2.0336 -2.4164
H 0.1088 -1.0169 -3.8630
H -2.1710 1.0051 -1.9011

[Pd](C2H4)CH3+
160 -433.161124
Pd 0.0253 -0.0023 0.0033
N -0.0271 0.0094 2.2875
N 2.0593 -0.0026 0.6218
C 1.1424 0.0102 2.8081
C 2.3035 0.0021 1.8797
H -0.7869 0.0159 2.9714
H 2.8786 -0.0080 0.0119
H 3.3162 0.0006 2.2839
H 1.3287 0.0164 3.8831
C 0.5210 -0.0124 -1.9643
H -0.3478 -0.0638 -2.6208
H 1.0723 0.9167 -2.1392
H 1.1620 -0.8865 -2.1116
C -2.0446 0.6861 -0.5194
C -2.0501 -0.6903 -0.4929
H -1.9625 1.2317 -1.4550
H -2.3487 1.2675 0.3475
H -2.3591 -1.2354 0.3956
H -1.9726 -1.2724 -1.4067

[Pd](C2H4)CH2CH2CH3+
208 -511.794756
Pd -0.1247 -0.0287 0.0006

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N 0.1273 0.1162 2.2895
N 1.9835 0.1949 0.3583
C 1.3491 0.2392 2.6479
C 2.3778 0.2822 1.5743
H -0.5325 0.0888 3.0699
H 2.7263 0.2245 -0.3422
H 3.4285 0.3851 1.8477
H 1.6739 0.3136 3.6870
C 0.0734 -0.0872 -2.0369
H 0.8918 -0.8010 -2.1930
H -0.8374 -0.5028 -2.4760
C 0.3853 1.2937 -2.6006
H 1.2972 1.7039 -2.1484
H -0.4223 1.9959 -2.3645
C 0.5636 1.2351 -4.1323
H 0.7902 2.2299 -4.5268
H -0.3482 0.8779 -4.6215
H 1.3816 0.5642 -4.4127
C -2.3217 0.3122 -0.2308
C -2.1181 -1.0452 -0.1180
H -2.4696 0.7810 -1.1990
H -2.5873 0.9135 0.6352
H -2.2089 -1.5520 0.8395
H -2.0932 -1.6858 -0.9947

[Pd](C2H4)CH(CH3)2+
208 -511.796392
Pd -0.0507 0.0897 -0.0736
N -0.0740 0.0169 2.2571
N 1.9796 0.4671 0.5880
C 1.0769 0.2222 2.7745
C 2.2135 0.4680 1.8474
H -0.8131 -0.1425 2.9452
H 2.7983 0.6394 0.0028
H 3.2073 0.6407 2.2626
H 1.2703 0.2281 3.8488
C 0.3302 0.2542 -2.0987
H -0.6125 0.0177 -2.6007
C 0.7106 1.7032 -2.3605
C 1.3861 -0.7698 -2.4845
H 1.0888 -1.7923 -2.2338
H 2.3598 -0.5713 -2.0249
H 1.5376 -0.7343 -3.5731
H 0.8656 1.8454 -3.4401
H 1.6446 1.9898 -1.8657
H -0.0707 2.4042 -2.0520
C -2.2451 0.2548 -0.4812
C -1.9075 -1.0804 -0.5148
H -2.3624 0.8302 -1.3953
H -2.6467 0.7103 0.4206
H -2.0295 -1.7137 0.3603
H -1.7454 -1.5977 -1.4562

[Pd]{O(CH3)2}CH3+
178 -509.592960
Pd -0.0076 -0.0000 -0.0014
N 0.0065 -0.0264 2.2814
N 1.9609 0.0074 0.4970
C 1.2052 -0.0193 2.7359
C 2.2975 -0.0074 1.7376
H -0.7135 -0.0323 3.0061
H 2.7273 0.0134 -0.1777
H 3.3390 -0.0109 2.0570
H 1.4565 -0.0211 3.7971
C 0.4262 0.0372 -1.9783
H -0.5172 -0.0166 -2.5222
H 0.9558 0.9698 -2.1948
H 1.0541 -0.8300 -2.2038
O -2.0866 -0.0367 -0.5586
C -2.8996 -1.1477 -0.1366
H -3.7559 -1.2375 -0.8131
H -2.2809 -2.0427 -0.2043
H -3.2509 -1.0020 0.8915
C -2.8163 1.2030 -0.6434
H -3.1480 1.5243 0.3506
H -2.1425 1.9428 -1.0757
H -3.6817 1.0612 -1.2989

[Pd]{O(CH3)2}CH2CH2CH3+
226 -588.226473
Pd 0.0620 0.0223 0.0105
N -0.0426 -0.0978 2.3211
N 1.9898 0.2330 0.6445
C 1.1233 0.0315 2.8370
C 2.2574 0.2019 1.9015
H -0.7894 -0.2020 3.0107
H 2.7912 0.3534 0.0233
H 3.2734 0.2998 2.2824
H 1.3209 0.0269 3.9099
C 0.5708 0.1755 -1.9572
H -0.1476 0.8984 -2.3608
H 1.5742 0.6128 -2.0100
C 0.4901 -1.1684 -2.6677
H 1.1984 -1.8794 -2.2250
H -0.5117 -1.5961 -2.5469
C 0.7930 -1.0244 -4.1738
H 0.0756 -0.3549 -4.6593
H 1.7969 -0.6214 -4.3416
H 0.7339 -1.9982 -4.6693
O -1.9806 -0.2126 -0.6822
C -2.7192 -1.3688 -0.2482
H -3.5325 -1.5597 -0.9565
H -2.9274 -2.2115 0.2469
C -2.8120 0.9532 -0.8388
H -3.2247 1.2653 0.1275
H -2.1861 1.7434 -1.2532
H -3.6250 0.7206 -1.5348

[Pd]{O(CH3)2}CH(CH3)2+
226 -588.227739
Pd -0.0160 0.0045 -0.0026
N 0.0226 0.0119 2.3268
N 1.9753 0.0330 0.5139
C 1.2271 0.0351 2.7625
C 2.3116 0.0422 1.7543
H -0.6816 0.0095 3.0672
H 2.7504 0.0396 -0.1502
H 3.3528 0.0575 2.0753
H 1.4948 0.0513 3.8202
C 0.3360 -0.0279 -2.0299
C 0.9739 -1.3553 -2.4085
H -0.6921 0.0203 -2.4038
C 1.1219 1.1974 -2.4691
H 0.6596 2.1335 -2.1424
H 2.1593 1.1863 -2.1158
H 1.1690 1.2241 -3.5676
H 1.9935 -1.4588 -2.0203
H 1.0429 -1.4263 -3.5041
H 0.3881 -2.2136 -2.0666
O -2.1453 -0.0306 -0.4930
C -2.9640 -1.0641 0.0816
H -3.8657 -1.1879 -0.5280
H -2.3796 -1.9843 0.0654
H -3.2453 -0.8094 1.1105
C -2.8423 1.2206 -0.6386
H -3.0951 1.6391 0.3426
H -2.1785 1.8978 -1.1766
H -3.7556 1.0577 -1.2211

[Pd](NCCH3)CH3+
172 -487.338817
Pd -0.1712 -0.2276 0.0000
N 2.0902 -0.2419 0.0000
N 0.3353 -2.2114 0.0000
C 2.5650 -1.4323 0.0000
C 1.5791 -2.5367 0.0000
H 2.7939 0.4984 0.0000
H -0.3286 -2.9871 0.0000
H 1.9117 -3.5742 0.0000
H 3.6303 -1.6666 0.0000
C -2.1543 -0.6776 0.0000
H -2.3447 -1.2660 -0.9023
H -2.3447 -1.2660 0.9023
H -2.7583 0.2282 0.0000
N -0.6443 1.7521 0.0000
C -0.9385 2.8698 0.0000
C -1.3112 4.2781 0.0000
H -1.9048 4.5041 0.8919
H -1.9048 4.5041 -0.8919
H -0.4124 4.9032 0.0000

[Pd](NCCH3)CH2CH2CH3+
220 -565.971702
Pd 0.0548 0.0347 0.0273
N 0.0076 -0.0636 2.3153
N 2.0180 0.1945 0.6154
C 1.1805 0.0316 2.8209
C 2.3057 0.1678 1.8679
H -0.7439 -0.1511 3.0017
H 2.8140 0.2902 -0.0169
H 3.3292 0.2425 2.2340
H 1.3895 0.0198 3.8915
C 0.5290 0.1709 -1.9619
H -0.2040 0.8578 -2.3952
H 1.5143 0.6503 -1.9989
C 0.5250 -1.1887 -2.6511
H -0.4586 -1.6615 -2.5494
H 1.2449 -1.8639 -2.1725
C 0.8706 -1.0576 -4.1477
H 1.8621 -0.6159 -4.2910
H 0.1438 -0.4244 -4.6673
H 0.8674 -2.0401 -4.6295
N -1.9077 -0.1268 -0.5290
C -3.0041 -0.2206 -0.8832
C -4.3820 -0.3394 -1.3418
H -4.4453 -1.0995 -2.1273
H -4.7223 0.6199 -1.7448
H -5.0312 -0.6295 -0.5098

[Pd](NCCH3)CH(CH3)2+
220 -565.972405
Pd -0.0032 0.0022 -0.0045
N 0.0115 0.0143 2.3023
N 1.9965 0.0128 0.5411
C 1.2022 0.0270 2.7721
C 2.3089 0.0286 1.7874
H -0.7227 0.0095 3.0126
H 2.7864 0.0158 -0.1051
H 3.3430 0.0437 2.1307
H 1.4417 0.0357 3.8368
C 0.3718 -0.0242 -2.0411
H -0.6261 0.0206 -2.4852
C 1.1615 1.2137 -2.4374
H 1.2547 1.2463 -3.5326
H 2.1822 1.2176 -2.0388
H 0.6674 2.1381 -2.1254
H 2.0327 -1.4532 -1.9461
H 1.1655 -1.4131 -3.4803
H 0.4326 -2.2062 -2.0820
N -2.0103 0.0132 -0.4317
C -3.1360 0.0321 -0.6963
C -4.5519 0.0583 -1.0412
H -4.7777 -0.7516 -1.7424
H -4.8012 1.0158 -1.5101
H -5.1608 -0.0684 -0.1406

[Pd]{S(CH3)2}CH3+
190 -832.621337
Pd -0.0139 0.0428 0.0421
N 0.1536 -0.5858 2.1899
N 1.9969 0.3161 0.5341
C 1.3468 -0.4903 2.6512
C 2.3812 0.0179 1.7220
H -0.5251 -0.9440 2.8638
H 2.7225 0.6651 -0.0941
H 3.4134 0.1256 2.0543
H 1.6265 -0.7592 3.6704
C 0.3069 0.6759 -1.8738
H 1.2130 0.1647 -2.2115
H 0.4653 1.7577 -1.8240
H -0.5090 0.4397 -2.5586
S -2.2693 -0.3268 -0.5960
C -3.1941 -0.8249 0.8984
H -4.2522 -0.9082 0.6368
H -2.8264 -1.8087 1.1978
H -3.0653 -0.1022 1.7074
C -3.0195 1.3159 -0.8999
H -2.9113 1.9670 -0.0306
H -2.5097 1.7535 -1.7597
H -4.0751 1.1692 -1.1420

[Pd]{S(CH3)2}CH2CH2CH3+
238 -911.253590
Pd 0.0301 -0.0106 0.0583
N 0.0927 -0.3037 2.3345
N 2.0226 0.2998 0.6205
C 1.2666 -0.1260 2.8170
C 2.3473 0.1995 1.8580
H -0.6120 -0.5205 3.0415
H 2.7882 0.5231 -0.0176
H 3.3670 0.3436 2.2149
H 1.5052 -0.1994 3.8791
C 0.4414 0.3394 -1.9287
H -0.3892 0.9097 -2.3584
H 1.3210 0.9936 -1.9132
C 0.6952 -0.9486 -2.7037
H 1.5235 -1.5091 -2.2528
H -0.1857 -1.5992 -2.6559
C 1.0221 -0.6570 -4.1819
H 0.1940 -0.1355 -4.6730
H 1.9167 -0.0331 -4.2782
H 1.2011 -1.5895 -4.7255
S -2.2219 -0.3926 -0.6563
C -3.1553 -1.0543 0.7664
H -4.2019 -1.1702 0.4727
H -2.7397 -2.0365 1.0008
H -3.0810 -0.3923 1.6321
C -3.0172 1.2472 -0.8239
H -2.9392 1.8215 0.1011
H -2.5104 1.7763 -1.6330
H -4.0649 1.0957 -1.0955

[Pd]{S(CH3)2}CH(CH3)2+
238 -911.253829
Pd -0.0430 -0.0941 -0.0196
N -0.0147 -0.2855 2.2674
N 1.9972 -0.1377 0.5426
C 1.1712 -0.3353 2.7491
C 2.2936 -0.2498 1.7862
H -0.7489 -0.3501 2.9746
H 2.7976 -0.0801 -0.0884
H 3.3210 -0.2834 2.1488
H 1.3920 -0.4355 3.8131
C 0.3452 0.0202 -2.0608
C 0.9858 -1.2932 -2.4867
H -0.6272 0.1137 -2.5560
C 1.1761 1.2633 -2.3467
H 0.6899 2.1798 -1.9983
H 2.1757 1.2192 -1.9013
H 1.3205 1.3635 -3.4324
H 1.9587 -1.4643 -2.0137
H 1.1585 -1.2794 -3.5730
H 0.3443 -2.1525 -2.2714
S -2.3542 -0.1523 -0.6258
C -3.3514 -0.3283 0.8929
H -4.4094 -0.2873 0.6206
H -3.1317 -1.3116 1.3144
H -3.1219 0.4590 1.6147
C -2.8407 1.5394 -1.1277
H -2.6430 2.2613 -0.3330
H -2.2612 1.7976 -2.0161
H -3.9030 1.5319 -1.3845

[Pd](Cl)CH3
146 -815.001667
Pd 0.0130 -0.0051 -0.0402
N -0.0087 -0.0032 2.1819
N 1.9883 -0.0030 0.4969
C 1.1668 -0.0001 2.7019
H -0.7940 -0.0009 2.8336
H 2.7806 -0.0058 -0.1457
H 3.3187 -0.0036 2.1128
H 1.3642 0.0042 3.7753
C 0.4004 0.0025 -2.0328
H -0.5298 -0.0560 -2.5965
H 0.9273 0.9359 -2.2599
H 1.0362 -0.8630 -2.2506
Cl -2.2793 -0.0087 -0.4108

[Pd](Cl)CH2CH2CH3
194 -893.633120
Pd 0.0136 -0.0047 -0.0282
N 0.0063 0.0080 2.2143
N 1.9920 -0.0483 0.5106
C 1.1862 -0.0077 2.7226
C 2.3010 -0.0420 1.7672
H -0.7693 0.0357 2.8768
H 2.7827 -0.0682 -0.1345
H 3.3323 -0.0583 2.1186
H 1.3951 0.0044 3.7940
C 0.3649 -0.0101 -2.0427
H -0.3081 0.7402 -2.4670
H 1.4018 0.3321 -2.1762
C 0.1443 -1.3778 -2.6841
H 0.8068 -2.1261 -2.2280
H -0.8817 -1.7063 -2.4899
C 0.3913 -1.3492 -4.2047
H -0.2867 -0.6438 -4.6976
H 1.4176 -1.0424 -4.4393
H 0.2276 -2.3373 -4.6498
Cl -2.2829 0.0627 -0.4065

[Pd](Cl)CH(CH3)2
194 -893.632865
Pd 0.0168 -0.0069 -0.0236
N 0.0057 0.0311 2.2269
N 2.0017 -0.0353 0.5312
C 1.1828 0.0185 2.7400
C 2.3022 -0.0203 1.7890
H -0.7733 0.0575 2.8856
H 2.7994 -0.0624 -0.1041
H 3.3312 -0.0359 2.1473
H 1.3876 0.0339 3.8125
C 0.3478 -0.0416 -2.0580
C 1.0047 -1.3604 -2.4516
H -0.6568 0.0094 -2.4834
C 1.1453 1.1881 -2.4808
H 0.6394 2.1165 -2.2008
H 2.1556 1.2111 -2.0514
H 1.2706 1.1966 -3.5750
H 1.9990 -1.4909 -2.0044
H 1.1426 -1.4017 -3.5438
H 0.3913 -2.2192 -2.1651
Cl -2.2906 0.0206 -0.3647

F4. "real" compounds, (diimine) = acenaphtylene (NAr)2, C36H40N2

[Pd]CH3+
502 -1671.618645
Pd 0.0011 0.0032 0.0467
N -0.0025 0.0113 2.2358
N 2.0497 0.0026 0.4094
C 1.2023 0.0071 2.6901
C 2.3336 0.0011 1.6749
C -1.1844 0.0693 3.0571
C -1.9807 -1.1017 3.1468
C -3.1689 -1.0319 3.8898
C -3.5715 0.1627 4.4941
C -2.7911 1.3141 4.3585
C -1.5837 1.3008 3.6398
H -3.7869 -1.9171 3.9910
H -4.4969 0.1993 5.0593
H -3.1278 2.2415 4.8089
C 3.0733 -0.0224 -0.6114
C 3.4981 1.2071 -1.1767
C 4.4924 1.1564 -2.1668
C 5.0251 -0.0628 -2.5964
C 4.5608 -1.2623 -2.0495
C 3.5709 -1.2751 -1.0527
H 4.8482 2.0804 -2.6091
H 5.7917 -0.0784 -3.3640
H 4.9667 -2.2037 -2.4041
C 0.0886 0.0236 -1.9631
H 0.3272 1.0362 -2.2994
H 0.8157 -0.6910 -2.3508
H -0.9366 -0.2579 -2.2510
C 4.9432 -0.0101 2.0811
C 3.5946 -0.0085 2.4216
C 3.2255 -0.0215 3.8030
C 4.1688 -0.0504 4.8517
C 5.5441 -0.0517 4.4704
C 5.9067 -0.0291 3.1265
H 5.2699 0.0004 1.0491
C 1.8159 -0.0103 4.0239
C 3.6437 -0.0778 6.1793
H 6.3121 -0.0710 5.2372
H 6.9580 -0.0294 2.8610
C 2.2697 -0.0765 6.3965
C 1.3327 -0.0407 5.3256
H 4.3256 -0.1017 7.0235
H 0.2707 -0.0365 5.5379
C -0.9197 -3.3764 3.5331
C -1.5454 -2.4144 2.4918
H -0.0680 -2.9143 4.0455
H -1.6589 -3.6549 4.2936
H -0.5711 -4.2945 3.0463
C -2.6943 -3.1057 1.7240
H -0.7626 -2.1765 1.7569
H -3.1534 -2.4277 0.9950
H -2.3122 -3.9807 1.1862
H -3.4824 -3.4557 2.3997
C -1.5245 3.5099 2.4064
C -0.8046 2.6037 3.4380
H -1.6501 2.9970 1.4449
H -2.5194 3.7967 2.7655
H -0.9477 4.4259 2.2339
C -0.5627 3.3654 4.7611
H 0.1800 2.3611 3.0233
H -0.0493 2.7367 5.4968
H 0.0583 4.2491 4.5757
H -1.5016 3.7118 5.2068
C 2.4074 -3.4648 -1.6151
C 3.0667 -2.6124 -0.5029
H 1.5759 -2.9318 -2.0893
H 3.1296 -3.7256 -2.3968
H 2.0184 -4.3987 -1.1937
C 4.1964 -3.4084 0.1953
H 2.2954 -2.4083 0.2486
H 4.6503 -2.8320 1.0086
H 3.7983 -4.3387 0.6160
H 4.9885 -3.6752 -0.5138
C 3.9304 3.3341 0.1522
C 2.9234 2.5544 -0.7311
H 4.2187 2.7604 1.0397
H 4.8421 3.5650 -0.4113
H 3.4904 4.2815 0.4844
C 2.4729 3.4216 -1.9299
H 2.0325 2.3564 -0.1218
H 1.7709 2.8624 -2.5751
H 1.9785 4.3303 -1.5686
H 3.3237 3.7330 -2.5460

[Pd]CH2CH2CH3+
550 -1750.268614
Pd 0.8105 0.1015 -0.8046
N 0.2861 0.3840 1.3072
N 2.6890 0.5786 0.0298
C 1.3183 0.6778 2.0207
C 2.6572 0.7858 1.3041
C -1.0481 0.2862 1.8516
C -1.5724 -1.0026 2.1057
C -2.8957 -1.0922 2.5682
C -3.6777 0.0559 2.7473
C -3.1428 1.3173 2.4607
C -1.8192 1.4638 2.0069
H -3.3169 -2.0676 2.7862
H -4.6998 -0.0333 3.1008
H -3.7619 2.1997 2.5856
C 3.9087 0.6618 -0.7516
C 4.2376 1.8940 -1.3704
C 5.4064 1.9417 -2.1478
C 6.2091 0.8092 -2.3185
C 5.8464 -0.4014 -1.7205
C 4.6886 -0.5051 -0.9309
H 5.6879 2.8740 -2.6248
H 7.1078 0.8677 -2.9215
H 6.4663 -1.2786 -1.8699
C 1.1422 -0.1727 -2.7995
H 1.5103 0.7416 -3.2656
H 1.7885 -1.0352 -2.9616
C -0.3215 -0.3929 -2.8114
H -0.6076 -1.4296 -3.0126
H -0.7039 -0.3191 -1.6650
C -1.1916 0.6247 -3.5551
H -0.8997 1.6471 -3.3003
H -1.0623 0.4896 -4.6312
H -2.2536 0.4972 -3.3187
C 5.0374 1.3784 2.2822
C 3.6679 1.1363 2.3080
C 2.9701 1.2182 3.5514
C 3.6084 1.5287 4.7729
C 5.0150 1.7707 4.7161
C 5.6961 1.6975 3.5038
H 5.6068 1.3274 1.3634
C 1.5680 0.9582 3.4430
C 2.7761 1.5680 5.9315
H 5.5544 2.0143 5.6267
H 6.7637 1.8872 3.4830
C 1.4097 1.3122 5.8294
C 0.7823 1.0068 4.5868
H 3.2161 1.8006 6.8963
H 0.7960 1.3472 6.7218
H -0.2835 0.8173 4.5516
C -0.3372 -2.8984 3.2668
C -0.7315 -2.2671 1.9113
H 0.2084 -2.1874 3.8929
H -1.2257 -3.2199 3.8186
H 0.3016 -3.7766 3.1124
C -1.4391 -3.2987 1.0070
H 0.1942 -1.9790 1.4065
H -1.7163 -2.8568 0.0429
H -0.7734 -4.1510 0.8203
H -2.3536 -3.6869 1.4721
C -1.2806 2.8516 1.6445
H -1.8379 2.6998 -0.4772
H -3.0487 3.5216 0.5248
H -1.5505 4.3611 0.0894
C -1.4138 3.8640 2.8081
H -0.2127 2.7614 1.4166
H -0.9060 3.5033 3.7110
H -0.9640 4.8209 2.5243
H -2.4642 4.0521 3.0612
C 4.1230 -2.9401 -1.4038
C 4.3036 -1.8495 -0.3135
H 3.3764 -2.6356 -2.1512
H 5.0624 -3.1448 -1.9339
H 3.7940 -3.8786 -0.9459
C 5.3356 -2.3087 0.7501
H 3.3378 -1.7226 0.1882
H 5.4413 -1.5640 1.5493
H 5.0225 -3.2543 1.2017
H 6.3241 -2.4712 0.3038
C 4.0875 4.2360 -0.3869
C 3.3709 3.1462 -1.2155
H 4.3655 3.8642 0.6021
H 4.9978 4.5728 -0.8885
H 3.4356 5.1063 -0.2591
C 2.9383 3.7145 -2.5867
H 2.4640 2.8633 -0.6748
H 2.4126 2.9611 -3.1827
H 2.2702 4.5707 -2.4480
H 3.7985 4.0569 -3.1691

[Pd]CH(CH3)2+
550 -1750.271337
Pd 0.7570 0.2191 -0.8314
N 0.2994 0.3576 1.3185
N 2.6907 0.5848 -0.0016
C 1.3406 0.6631 2.0094
C 2.6691 0.7818 1.2757
C -1.0203 0.2237 1.8916
C -1.5110 -1.0816 2.1379
C -2.8213 -1.2081 2.6270
C -3.6248 -0.0843 2.8397
C -3.1279 1.1920 2.5603
C -1.8199 1.3787 2.0800
H -3.2159 -2.1958 2.8395
H -4.6361 -0.2029 3.2142
H -3.7645 2.0573 2.7115
C 3.9272 0.5829 -0.7533
C 4.2470 1.7254 -1.5318
C 5.4315 1.6943 -2.2856
C 6.2589 0.5667 -2.2849
C 5.9079 -0.5573 -1.5332
C 4.7375 -0.5821 -0.7534
H 5.7080 2.5580 -2.8797
H 7.1699 0.5622 -2.8743
H 6.5479 -1.4332 -1.5521
C 0.9518 0.1634 -2.8770
H 1.2338 1.1700 -3.1916
C -0.5114 -0.0666 -2.7599
H -0.8503 -1.0489 -3.0951
H -0.8446 -0.0804 -1.6208
C 5.0555 1.3800 2.2393
C 3.6900 1.1206 2.2751
C 3.0017 1.1947 3.5253
C 3.6449 1.5058 4.7423
C 5.0469 1.7638 4.6735
C 5.7181 1.7038 3.4559
H 5.6186 1.3383 1.3158
C 1.6028 0.9276 3.4307
C 2.8223 1.5299 5.9090
H 5.5911 2.0097 5.5798
H 6.7829 1.9065 3.4267
C 1.4607 1.2596 5.8203
C 0.8267 0.9570 4.5823
H 3.2669 1.7616 6.8717
H 0.8559 1.2816 6.7199
H -0.2375 0.7589 4.5557
C -0.2318 -2.9812 3.2417
C -0.6509 -2.3252 1.9027
H 0.3127 -2.2755 3.8786
H -1.1106 -3.3284 3.7980
H 0.4156 -3.8466 3.0583
C -1.3556 -3.3491 0.9824
H 0.2666 -2.0080 1.3906
H -1.6406 -2.8945 0.0254
H -0.6884 -4.1935 0.7767
H -2.2645 -3.7505 1.4463
C -2.0378 3.3040 0.4466
C -1.3312 2.7861 1.7240
H -1.8712 2.6270 -0.3998
H -3.1192 3.3865 0.6020
H -1.6575 4.2955 0.1746
C -1.5065 3.7847 2.8906
H -0.2599 2.7346 1.5009
H -0.9937 3.4355 3.7926
H -1.0898 4.7610 2.6177
H -2.5624 3.9343 3.1370
C 4.1298 -3.0464 -0.9302
C 4.3829 -1.8542 0.0245
H 3.3284 -2.8247 -1.6412
H 5.0303 -3.2924 -1.5026
H 3.8440 -3.9358 -0.3565
C 5.4715 -2.2191 1.0619
H 3.4517 -1.6777 0.5732

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H 5.1669 -3.1044 1.6318
H 6.4232 -2.4502 0.5719
C 3.8818 4.0316 -0.5258
C 3.3572 2.9710 -1.5267
H 3.9474 3.6311 0.4906
H 4.8814 4.3730 -0.8182
H 3.2168 4.9027 -0.5087
C 3.1902 3.5952 -2.9289
H 2.3595 2.6629 -1.1862
H 2.8668 2.8523 -3.6659
H 2.4421 4.3952 -2.8944
H 4.1237 4.0391 -3.2903
C 1.8391 -0.9179 -3.4418
H 2.8859 -0.7428 -3.1785
H 1.5483 -1.9120 -3.0898
H 1.7779 -0.9237 -4.5391
H -1.1433 0.7355 -3.1455

[Pd](C2H4)CH3+
536 -1750.253065
Pd -0.0361 0.0373 0.0114
N -0.0028 -0.0365 2.2652
N 2.0769 -0.0710 0.4365
C 1.2041 -0.1117 2.7076
C 2.3473 -0.1367 1.6993
C -1.1434 0.0557 3.1477
C -1.8948 -1.1203 3.4079
C -3.0334 -1.0030 4.2217
C -3.4255 0.2334 4.7441
C -2.6870 1.3818 4.4504
C -1.5360 1.3262 3.6443
H -3.6205 -1.8862 4.4462
H -4.3093 0.3019 5.3699
H -3.0079 2.3392 4.8474
C 3.1364 -0.0819 -0.5535
C 3.6468 1.1566 -1.0165
C 4.6679 1.1208 -1.9814
C 5.1488 -0.0921 -2.4824
C 4.5997 -1.2983 -2.0383
C 3.5770 -1.3236 -1.0748
H 5.0859 2.0531 -2.3458
H 5.9394 -0.0969 -3.2254
H 4.9641 -2.2343 -2.4483
C 0.2384 0.1052 -2.0073
H 1.1327 0.7064 -2.1784
H 0.4089 -0.9269 -2.3282
H -0.6183 0.5288 -2.5347
C 4.9501 -0.2762 2.1359
C 3.5991 -0.2228 2.4629
C 3.2173 -0.2491 3.8393
C 4.1484 -0.3348 4.8967
C 5.5263 -0.3886 4.5290
C 5.9022 -0.3581 3.1895
H 5.2879 -0.2587 1.1079
C 1.8073 -0.1831 4.0473
C 3.6111 -0.3596 6.2189
H 6.2846 -0.4540 5.3029
H 6.9549 -0.3996 2.9328
C 2.2365 -0.3016 6.4241
C 1.3125 -0.2115 5.3456
H 4.2836 -0.4251 7.0684
H 1.8495 -0.3241 7.4368
H 0.2503 -0.1668 5.5504
C -0.6142 -3.2682 3.8960
C -1.4632 -2.4854 2.8606
H 0.2812 -2.7124 4.1914
H -1.2020 -3.4671 4.8001
H -0.2974 -4.2312 3.4787
C -2.6538 -3.3545 2.3955
H -0.8246 -2.3036 1.9847
H -3.3177 -2.8131 1.7117
H -2.2833 -4.2469 1.8790
H -3.2588 -3.6973 3.2422
C -1.6650 3.6584 2.6154
C -0.7705 2.6186 3.3346
H -2.0806 3.2605 1.6832
H -2.5023 3.9710 3.2492
H -1.0802 4.5524 2.3706
C -0.1569 3.2401 4.6137
H 0.0556 2.3773 2.6555
H 0.5139 2.5393 5.1206
H 0.4167 4.1389 4.3595
H -0.9402 3.5327 5.3225
C 2.4147 -3.4561 -1.8408
C 2.9785 -2.6639 -0.6365
H 1.6761 -2.8676 -2.3962
H 3.2092 -3.7413 -2.5394
H 1.9310 -4.3764 -1.4936
C 4.0039 -3.5231 0.1439
H 2.1386 -2.4588 0.0383
H 4.3782 -2.9975 1.0289
H 3.5414 -4.4608 0.4728
H 4.8635 -3.7767 -0.4877
C 4.1855 3.2094 0.3923
C 3.1323 2.5033 -0.4979
H 4.4743 2.5863 1.2456
H 5.0914 3.4361 -0.1822
H 3.7862 4.1548 0.7775
C 2.6859 3.4343 -1.6503
H 2.2487 2.3124 0.1239
H 1.9286 2.9566 -2.2818
H 2.2586 4.3575 -1.2423
H 3.5295 3.7153 -2.2905
C -2.1056 0.8005 -0.2088
H -2.3894 -1.2342 0.4112
H -2.1540 -0.9931 -1.4028
H -2.3336 1.2202 0.7668
H -2.0985 1.4939 -1.0448

[Pd](C2H4)CH2CH2CH3+
586 -1828.882869
Pd -0.0516 -0.0260 0.0059
N -0.0041 -0.0138 2.2873
N 2.0829 -0.0036 0.4556
C 1.2047 -0.0020 2.7279
C 2.3493 -0.0082 1.7209
C -1.1427 0.0568 3.1734
C -1.8252 -1.1447 3.4984
C -2.9628 -1.0511 4.3167
C -3.4216 0.1860 4.7799
C -2.7527 1.3582 4.4198
C -1.6060 1.3267 3.6065
H -3.4973 -1.9537 4.5904
H -4.3034 0.2360 5.4101
H -3.1262 2.3152 4.7693
C 3.1589 0.0018 -0.5160
C 3.6432 1.2467 -0.9907
C 4.6847 1.2246 -1.9341
C 5.2115 0.0181 -2.4037
C 4.6872 -1.1961 -1.9513
C 3.6443 -1.2348 -1.0100
H 5.0820 2.1628 -2.3068
H 6.0180 0.0240 -3.1295
H 5.0867 -2.1277 -2.3378
C 0.2592 -0.0443 -2.0332
H 1.2989 0.2862 -2.0977
H 0.2141 -1.1122 -2.2827
C -0.6288 0.7858 -2.9516
C -0.1295 0.7168 -4.4079
H -0.6360 1.8345 -2.6270
H -1.6685 0.4375 -2.9258
H -0.7682 1.3165 -5.0642
H -0.1362 -0.3135 -4.7795
H 0.8941 1.0964 -4.4939
C 4.9561 -0.0004 2.1655
C 3.6031 0.0009 2.4889
C 3.2206 0.0154 3.8651
C 4.1524 0.0233 4.9257
C 5.5321 0.0218 4.5612
C 5.9088 0.0110 3.2219
H 5.2960 -0.0111 1.1382
C 1.8090 0.0190 4.0698
C 3.6141 0.0307 6.2476
H 6.2909 0.0286 5.3374
H 6.9628 0.0098 2.9671
C 2.2380 0.0290 6.4498
C 1.3132 0.0236 5.3679
H 4.2872 0.0367 7.0993
H 1.8500 0.0328 7.4624
H 0.2497 0.0238 5.5703
C -0.4480 -3.2104 4.0774
C -1.3246 -2.5080 3.0082
H 0.4183 -2.6022 4.3562
H -1.0324 -3.4026 4.9851
H -0.0834 -4.1725 3.6986
C -2.4699 -3.4488 2.5692
H -0.6882 -2.3294 2.1301
H -3.1544 -2.9628 1.8642
H -2.0553 -4.3410 2.0867
H -3.0634 -3.7891 3.4251
C -1.8764 3.5690 2.4216
C -0.9225 2.6424 3.2153
H -2.2536 3.0799 1.5167
H -2.7398 3.8661 3.0275
H -1.3503 4.4819 2.1195
C -0.3609 3.3863 4.4520
H -0.0770 2.4102 2.5575
H 0.3487 2.7644 5.0071
H 0.1568 4.3009 4.1405
H -1.1666 3.6752 5.1369
C 2.5887 -3.4269 -1.7663
C 3.0720 -2.5834 -0.5619
H 1.8657 -2.8741 -2.3758
H 3.4238 -3.7145 -2.4149
H 2.1105 -4.3478 -1.4133
C 4.0896 -3.3856 0.2866
H 2.1963 -2.3883 0.0692
H 4.4042 -2.8254 1.1736
H 3.6456 -4.3313 0.6183
H 4.9857 -3.6227 -0.2989
C 4.1132 3.3993 0.2916
C 3.0721 2.5873 -0.5179
H 4.4724 2.8374 1.1606
H 4.9807 3.6530 -0.3289
H 3.6705 4.3365 0.6482
C 2.5294 3.4238 -1.7017
H 2.2245 2.3813 0.1468
H 1.7735 2.8688 -2.2684
H 2.0705 4.3477 -1.3312
H 3.3307 3.7050 -2.3942
C -2.0939 -0.8285 -0.3911
C -2.2033 0.5204 -0.1298
H -2.2444 -1.5588 0.3979
H -2.0987 -1.2117 -1.4068
H -2.4434 0.8665 0.8715
H -2.2963 1.2471 -0.9295

[Pd](C2H4)CH(CH3)2+
586 -1828.878669
Pd -0.0632 -0.0171 -0.0494
N -0.0155 0.0174 2.2538
N 2.0906 0.0429 0.4280
C 1.1917 0.0366 2.6967
C 2.3424 0.0036 1.6953
C -1.1504 0.0607 3.1474
C -1.7303 -1.1601 3.5838
C -2.8493 -1.0849 4.4306
C -3.3861 0.1467 4.8167
C -2.8216 1.3338 4.3426
C -1.7029 1.3214 3.4915
H -3.3056 -2.0010 4.7893
H -4.2474 0.1803 5.4757
H -3.2550 2.2846 4.6341
C 3.1842 0.0488 -0.5252
C 3.7470 1.2893 -0.9248
C 4.8166 1.2532 -1.8357
C 5.2948 0.0439 -2.3493
C 4.6899 -1.1602 -1.9800
C 3.6170 -1.1860 -1.0723
H 5.2745 2.1837 -2.1521
H 6.1247 0.0425 -3.0484
H 5.0496 -2.0917 -2.4036
C 0.2480 0.0491 -2.1083
H 1.3036 -0.2383 -2.1090
H 0.5697 1.6045 -3.5651
C 0.1003 1.4922 -2.5765
C -0.5490 -0.9351 -2.9520
H 0.5889 2.2038 -1.9061
H -0.9468 1.7912 -2.6862
H -0.1719 -0.9057 -3.9847
H -1.6140 -0.6838 -3.0041
H -0.4473 -1.9666 -2.6020
C 4.9425 -0.1497 2.1589
C 3.5904 -0.0578 2.4734
C 3.2020 -0.0088 3.8465
C 4.1278 -0.0362 4.9123
C 5.5065 -0.1282 4.5567
C 5.8884 -0.1863 3.2202
H 5.2876 -0.1892 1.1342
C 1.7914 0.0654 4.0423
C 3.5850 0.0289 6.2307
H 6.2602 -0.1541 5.3374
H 6.9414 -0.2585 2.9715
C 2.2102 0.1096 6.4244
C 1.2912 0.1253 5.3376
H 4.2537 0.0143 7.0857
H 1.8182 0.1587 7.4342
H 0.2283 0.1808 5.5349
C -0.3195 -3.1564 4.3213
C -1.1593 -2.5260 3.1806
H 0.5132 -2.5120 4.6178
H -0.9438 -3.3312 5.2057
H 0.0909 -4.1213 4.0013
C -2.2559 -3.5217 2.7330
H -0.4888 -2.3681 2.3251
H -2.9027 -3.1016 1.9548
H -1.7919 -4.4321 2.3368
H -2.8957 -3.8198 3.5709
C -2.1900 3.5623 2.3561
C -1.1142 2.6429 2.9822
H -2.7463 3.0553 1.5597
H -2.9149 3.9019 3.1040
H -1.7173 4.4531 1.9271
C -0.3572 3.4006 4.1024
H -0.3888 2.4071 2.1932
H 0.4529 2.7963 4.5230
H 0.0761 4.3276 3.7090
H -1.0391 3.6674 4.9186
C 2.5649 -3.3376 -1.9523
C 2.9593 -2.5187 -0.7004
H 1.9387 -2.7517 -2.6335
H 3.4465 -3.6725 -2.5101
H 2.0058 -4.2320 -1.6538
C 3.8627 -3.3624 0.2334
H 2.0342 -2.2959 -0.1532
H 4.1038 -2.8249 1.1565
H 3.3612 -4.2991 0.5032
H 4.8054 -3.6165 -0.2659
C 4.1281 3.2103 0.7225
C 3.2302 2.6364 -0.4040
H 4.1958 2.5340 1.5792
H 5.1444 3.3861 0.3499
H 3.7276 4.1687 1.0732
C 3.0859 3.6856 -1.5326
H 2.2306 2.4686 0.0189
H 2.5227 3.2937 -2.3849
H 2.5646 4.5716 -1.1523
H 4.0638 4.0169 -1.8993
C -2.1149 -0.8881 -0.1396
C -2.2242 0.4734 -0.3172
H -2.2362 -1.3215 0.8475
H -2.1474 -1.5753 -0.9776
H -2.4355 1.1230 0.5277
H -2.3548 0.9062 -1.3028

[Pd]{O(CH3)2}CH3+
556 -1826.681552
Pd 0.0162 -0.0511 0.0345
N -0.0004 -0.0337 2.2800
N 2.0482 -0.0529 0.4486
C 2.3359 -0.1094 1.7113
C -1.1483 0.0951 3.1415
C -1.9946 -1.0328 3.3002
C -3.1493 -0.8846 4.0836
C -3.4710 0.3441 4.6695
C -2.6399 1.4495 4.4747
C -1.4635 1.3578 3.7094
H -3.8045 -1.7348 4.2349
H -4.3699 0.4403 5.2696
H -2.9065 2.4024 4.9202
C 3.1046 -0.0553 -0.5469
C 3.5653 1.1873 -1.0482
C 4.5915 1.1624 -2.0080
C 5.1222 -0.0461 -2.4682
C 4.6211 -1.2586 -1.9858
C 3.5978 -1.2944 -1.0230
H 4.9734 2.0987 -2.4007
H 5.9151 -0.0432 -3.2088
H 5.0236 -2.1919 -2.3651
C 0.2295 0.0060 -1.9849
H 1.2263 0.3557 -2.2506
H 0.0719 -1.0060 -2.3721
H -0.5322 0.6845 -2.3822
C 4.9473 -0.1895 2.1209
C 3.5983 -0.1716 2.4587
C 3.2290 -0.2235 3.8385
C 4.1699 -0.3124 4.8867
C 5.5457 -0.3294 4.5076
C 5.9094 -0.2654 3.1662
H 5.2770 -0.1513 1.0909
C 1.8200 -0.1851 4.0588
C 3.6430 -0.3783 6.2118
H 6.3116 -0.3933 5.2742
H 6.9606 -0.2781 2.9004
C 2.2691 -0.3558 6.4280
C 1.3352 -0.2565 5.3583
H 4.3233 -0.4490 7.0547
H 1.8906 -0.4118 7.4426
H 0.2735 -0.2359 5.5707
C -0.7975 -3.2470 3.6551
C -1.6309 -2.3812 2.6752
H 0.1162 -2.7333 3.9728
H -1.3826 -3.4802 4.5529
H -0.5106 -4.1933 3.1813
C -2.8615 -3.1698 2.1788
H -0.9982 -2.1745 1.8003
H -3.4982 -2.5534 1.5350
H -2.5375 -4.0479 1.6082
H -3.4746 -3.5344 3.0106
C -1.3750 3.6876 2.6846
C -0.6101 2.6139 3.4976
H -1.6734 3.3091 1.7004
H -2.2804 4.0129 3.2093
H -0.7412 4.5682 2.5289
C -0.1179 3.2118 4.8379
H 0.2758 2.3397 2.9144
H 0.4503 2.4795 5.4201
H 0.5306 4.0751 4.6495
H -0.9584 3.5549 5.4518
C 2.4072 -3.4257 -1.7250
C 3.0462 -2.6431 -0.5513
H 1.6183 -2.8400 -2.2092
H 3.1533 -3.6792 -2.4867
H 1.9692 -4.3623 -1.3608
C 4.1292 -3.4991 0.1488
H 2.2523 -2.4525 0.1800
H 4.5655 -2.9727 1.0044
H 3.6939 -4.4378 0.5105
H 4.9410 -3.7528 -0.5427
C 4.0185 3.3145 0.2747
C 2.9910 2.5258 -0.5745
H 4.3486 2.7361 1.1447
H 4.9050 3.5660 -0.3195
H 3.5769 4.2517 0.6329
C 2.4851 3.3851 -1.7575
H 2.1248 2.3149 0.0641
H 1.7434 2.8433 -2.3543
H 2.0188 4.3032 -1.3818
H 3.3050 3.6788 -2.4226
O -2.1233 -0.1824 -0.2529
C -2.8482 1.0575 -0.3293
H -3.9087 0.8642 -0.1342
H -2.4457 1.7098 0.4442
H -2.7256 1.5162 -1.3177
C -2.6583 -1.1808 -1.1402
H -2.5569 -0.8672 -2.1849
H -2.0967 -2.0981 -0.9666
H -3.7148 -1.3381 -0.8977

[Pd]{O(CH3)2}CH2CH2CH3+
604 -1905.312023
Pd 0.0963 -0.7236 -0.0111
N 0.0360 -0.2563 2.2036
N 2.0664 -0.0969 0.3410
C 1.2060 0.0947 2.6084
C 2.3247 0.1654 1.5840
C -1.1121 -0.2813 3.0754
C -1.5658 -1.5371 3.5535
C -2.7257 -1.5599 4.3445
C -3.4275 -0.3852 4.6327
C -2.9776 0.8376 4.1277
C -1.8155 0.9233 3.3408
H -3.0829 -2.5056 4.7376
H -4.3541 1.7430 4.3474
C 3.1335 -0.0577 -0.6416
C 3.3158 1.1248 -1.4020
C 4.3634 1.1429 -2.3381
C 5.1803 0.0249 -2.5317
C 4.9512 -1.1436 -1.8001
C 3.9226 -1.2167 -0.8447
H 4.5357 2.0378 -2.9256
H 5.9841 0.0604 -3.2597
H 5.5747 -2.0144 -1.9735
C 0.3415 -0.9748 -2.0213
H 1.3899 -0.7650 -2.2436
H 0.1486 -2.0376 -2.2160
H -0.5886 -0.0732 -2.8249
H -1.6371 -0.2816 -2.5795
H -0.4122 0.9775 -2.5641
C -0.3887 -0.2563 -4.3426
H 0.6381 -0.0124 -4.6350
H -0.5823 -1.2914 -4.6449
H -1.0652 0.3936 -4.9069
C 4.8726 0.7874 1.9388
C 3.5485 0.5576 2.2983
C 3.1680 0.7119 3.6672
C 4.0751 1.0779 4.6851
C 5.4254 1.3054 4.2838
C 5.7986 1.1634 2.9513
H 5.2108 0.6858 0.9158
H 1.7863 0.4570 3.9115
C 3.5443 1.1790 6.0063
H 6.1641 1.5904 5.0265
H 6.8298 1.3420 2.6672
C 2.1990 0.9226 6.2483
C 1.2979 0.5589 5.2079
H 4.1995 1.4568 6.8260
H 1.8171 1.0018 7.2601
H 0.2564 0.3735 5.4389
C 0.0606 -3.2649 4.4693
C -0.8010 -2.8298 3.2564
H 0.7701 -2.4825 4.7597
H -0.5744 -3.4828 5.3364
H 0.6295 -4.1710 4.2294
C -1.7324 -3.9804 2.8158
H -0.1187 -2.6269 2.4209
H -2.3646 -3.6744 1.9757
H -1.1374 -4.8468 2.5038
H -2.3868 -4.3105 3.6305
C -2.4433 2.8874 1.8418
C -1.3789 2.2878 2.7939
H -2.6330 2.2309 0.9852
H -3.3949 3.0496 2.3606
H -2.1029 3.8550 1.4554
C -1.0572 3.2871 3.9318
H -0.4631 2.1506 2.2082
H -0.2799 2.8996 4.5982
H -0.7047 4.2365 3.5122
H -1.9470 3.4991 4.5357
C 3.2410 -3.6519 -1.0664
C 3.6783 -2.5288 -0.0935
H 2.3444 -3.3636 -1.6262
H 4.0317 -3.8794 -1.7904
H 3.0214 -4.5706 -0.5098
C 4.9153 -2.9661 0.7278
H 2.8533 -2.3738 0.6109
H 4.6929 -3.8821 1.2872
H 5.7718 -3.1740 0.0761
C 3.1063 3.4285 -0.3339
C 2.4213 2.3533 -1.2157
H 3.3685 3.0372 0.6545
H 4.0275 3.7862 -0.8096
H 2.4409 4.2889 -0.1967
C 1.9820 2.9707 -2.5631
H 1.5122 2.0247 -0.6949
H 1.5366 2.2192 -3.2232
H 1.2402 3.7582 -2.3876
H 2.8247 3.4293 -3.0929
O -1.9005 -1.6335 -0.1066
C -3.0542 -0.7812 0.0004
H -3.9012 -1.3692 0.3713
H -2.8107 -0.0013 0.7196
H -3.3024 -0.3411 -0.9726
C -2.1534 -2.7919 -0.9176
H -2.3243 -2.5084 -1.9626
H -1.2789 -3.4373 -0.8398
H -3.0343 -3.3135 -0.5270

[Pd]{O(CH3)2}CH(CH3)2+
604 -1905.310027
Pd -0.0094 -0.1433 -0.0197
N -0.0526 -0.0852 2.2898
N 2.0472 -0.1104 0.4709
C 1.1527 -0.0727 2.7390
C 2.3009 -0.0751 1.7414
C -1.1945 -0.0404 3.1700
C -1.8889 -1.2537 3.4291
C -3.0417 -1.1926 4.2283
C -3.5019 0.0243 4.7431
C -2.8138 1.2061 4.4612
C -1.6501 1.2073 3.6701
H -3.5856 -2.1034 4.4503
H -4.3957 0.0495 5.3578
H -3.1823 2.1461 4.8589
C 3.1524 -0.1124 -0.4711
C 3.3335 1.0615 -1.2215
C 4.3809 1.0777 -2.1577
C 5.1977 -0.0350 -2.3713
C 4.9686 -1.2000 -1.6397
C 3.9398 -1.2031 -0.7035
H 4.5511 1.9844 -2.7262
H 6.0139 -0.0134 -3.1077
H 5.6023 -2.0824 -1.7995
C 0.3567 -0.9911 -1.8369
H 1.3997 -0.7888 -2.0966
H 0.1722 -2.0511 -2.0433
H -0.5660 -0.0900 -2.6511
H -1.6197 -0.2966 -2.3284
H -0.3911 0.9555 -2.3284
C 4.7381 1.0975 -1.8312
C 5.3255 -0.1115 -2.2157
C 4.7950 -1.3225 -1.7619
C 3.6916 -1.3540 -0.8920
H 5.1370 2.0303 -2.2142
H 6.1820 -0.1105 -2.8820
H 5.2377 -2.2562 -2.0911
C 0.2992 -0.2483 -2.0547
H 1.3888 -0.2608 -2.1350
C -0.2919 -1.5534 -2.5696
C -0.2730 0.9835 -2.7402
H -1.3662 0.9935 -2.7084
H 0.1002 1.9158 -2.3055
H 0.0186 0.9835 -3.8014
H -0.0200 -1.6909 -3.6273
H -1.3850 -1.5521 -2.5200
H 0.0836 -2.4260 -2.0264
C 4.9080 -0.0152 2.2057
C 3.5522 -0.0383 2.5172
C 3.1612 -0.0369 3.8914
C 4.0857 -0.0255 4.9589
C 5.4676 0.0001 4.6054
C 5.8527 0.0068 3.2689
H 5.2578 -0.0148 1.1820
C 1.7494 -0.0586 4.0864
C 3.5391 -0.0451 6.2772
H 6.2203 0.0131 5.3874
H 6.9082 0.0265 3.0208
C 2.1623 -0.0779 6.4697
C 1.2456 -0.0848 5.3810
H 4.2067 -0.0373 7.1331
H 1.7672 -0.0976 7.4794
H 0.1811 -0.1108 5.5762
C -0.3239 -3.2264 3.8414
C -1.3714 -2.5918 2.8886
H 0.5341 -2.5690 4.0072
H -0.7778 -3.4407 4.8164
H 0.0451 -4.1708 3.4241
C -2.4902 -3.6196 2.6097
H -0.8637 -2.3819 1.9351
H -3.2999 -3.1981 2.0050
H -2.0757 -4.4809 2.0737
H -2.9289 -3.9997 3.5393
C -1.8556 3.5332 2.6344
C -0.9388 2.5363 3.3847
H -2.2089 3.1185 1.6854
H -2.7333 3.7975 3.2351
H -1.3089 4.4585 2.4187
C -0.4047 3.1910 4.6830
H -0.0789 2.3352 2.7356
H 0.2806 2.5271 5.2184
H 0.1331 4.1160 4.4450
H -1.2272 3.4481 5.3606
C 2.8913 -3.6647 -1.6211
C 3.1115 -2.6964 -0.4348
H 2.3063 -3.1967 -2.4194
H 3.8424 -3.9982 -2.0512
H 2.3563 -4.5583 -1.2792
C 3.9948 -3.3726 0.6443
H 2.1289 -2.4994 0.0129
H 4.1146 -2.7390 1.5286
H 3.5464 -4.3216 0.9610
H 4.9935 -3.5883 0.2459
C 3.8195 3.2191 0.4916
C 2.9908 2.4639 -0.5786
H 3.9399 2.6293 1.4058
H 4.8196 3.4554 0.1086
H 3.3281 4.1632 0.7550
C 2.7620 3.3738 -1.8084
H 2.0055 2.2461 -0.1460
H 2.2237 2.8483 -2.6038
H 2.1763 4.2536 -1.5177
H 3.7088 3.7359 -2.2245
O -2.1793 -0.0793 -0.4696
C -2.8814 1.1573 -0.2784
H -3.1911 1.2622 0.7671
H -2.1993 1.9616 -0.5529
H -3.7620 1.1791 -0.9319
C -3.0149 -1.2113 -0.1912
H -3.8709 -1.2062 -0.8766
H -2.4149 -2.1055 -0.3570
H -3.3662 -1.1780 0.8455

[Pd](CH3CN)CH3+
550 -1804.426433
Pd 0.0302 0.0314 0.0120
N 0.0023 -0.0037 2.2435
N 2.0775 -0.0171 0.4500
C 1.2005 -0.0239 2.7114
C 2.3474 -0.0452 1.7167
C -1.1725 0.0024 3.0821
C -1.8177 -1.2307 3.3515
C -2.9950 -1.2007 4.1178
C -3.5274 0.0062 4.5809
C -2.8913 1.2120 4.2730
C -1.7077 1.2407 3.5151
H -3.4969 -2.1331 4.3549
H -4.4357 0.0071 5.1748
H -3.3174 2.1463 4.6239
C 3.1462 -0.0741 -0.5301
C 3.6122 1.1404 -1.0942
C 4.6364 1.0638 -2.0525
C 5.1597 -0.1689 -2.4534

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C 3.6316 -1.3373 -0.9459
H 5.0202 1.9774 -2.4937
H 5.9496 -0.2069 -3.1964
H 5.0464 -2.3062 -2.2492
C 0.2558 0.0452 -2.0156
H 1.3175 0.0282 -2.2569
H -0.2523 -0.8343 -2.4207
H -0.2169 0.9550 -2.3961
C 4.9497 -0.1318 2.1749
C 3.5956 -0.0990 2.4886
C 3.2022 -0.1045 3.8628
C 4.1246 -0.1506 4.9299
C 5.5068 -0.1856 4.5753
C 5.8936 -0.1740 3.2388
H 5.2966 -0.1264 1.1496
C 1.7893 -0.0602 4.0578
C 3.5745 -0.1570 6.2473
H 6.2594 -0.2212 5.3568
H 6.9491 -0.1989 2.9918
C 2.1972 -0.1180 6.4391
C 1.2813 -0.0681 5.3505
H 4.2400 -0.1928 7.1041
H 1.8019 -0.1248 7.4489
H 0.2160 -0.0370 5.5429
C -0.7178 -3.4257 4.0194
C -1.2623 -2.5670 2.8511
H 0.0628 -2.8944 4.5752
H -1.5185 -3.6814 4.7236
H -0.2914 -4.3614 3.6395
C -2.3100 -3.3569 2.0324
H -0.4235 -2.3538 2.1778
H -2.6763 -2.7649 1.1858
H -1.8648 -4.2773 1.6373
H -3.1713 -3.6425 2.6470
C -1.9911 3.4106 2.2306
C -1.0659 2.5838 3.1572
H -2.2278 2.8559 1.3152
H -2.9338 3.6589 2.7323
H -1.5039 4.3501 1.9451
C -0.6780 3.3948 4.4161
H -0.1446 2.3860 2.5980
H 0.0045 2.8282 5.0592
H -0.1800 4.3275 4.1274
H -1.5611 3.6587 5.0094
C 2.3437 -3.4395 -1.5454
C 3.0655 -2.6588 -0.4187
H 1.5434 -2.8403 -1.9929
H 3.0423 -3.7196 -2.3421
H 1.9029 -4.3603 -1.1455
C 4.1538 -3.5355 0.2450
H 2.3150 -2.4312 0.3471
H 4.6520 -3.0050 1.0637
H 3.7055 -4.4491 0.6522
H 4.9192 -3.8359 -0.4796
C 4.0303 3.2960 0.1912
C 3.0353 2.4993 -0.6887
H 4.3086 2.7368 1.0916
H 4.9491 3.5177 -0.3650
H 3.5860 4.2486 0.5027
C 2.6025 3.3335 -1.9170
H 2.1342 2.3175 -0.0903
H 1.8939 2.7800 -2.5422
H 2.1192 4.2607 -1.5879
H 3.4595 3.6121 -2.5407
N -1.9699 0.0618 -0.3270
C -3.1145 0.0693 -0.4878
C -4.5589 0.0716 -0.6818
H -5.0611 -0.0115 0.2873
H -4.8508 -0.7750 -1.3116
H -4.8687 1.0020 -1.1684

[Pd](CH3CN)CH2CH2CH3+
598 -1883.057288
Pd 0.0573 -0.6690 0.0240
N 0.0583 -0.2526 2.2277
N 2.0659 -0.1110 0.3519
C 1.2295 0.0997 2.6235
C 2.3414 0.1588 1.5890
C -1.0789 -0.3446 3.1104
C -1.4269 -1.6135 3.6379
C -2.5772 -1.6972 4.4404
C -3.3680 -0.5722 4.6926
C -3.0230 0.6613 4.1333
C -1.8790 0.8043 3.3290
H -2.8535 -2.6533 4.8728
H -4.2507 -0.6575 5.3182
H -3.6493 1.5276 4.3204
C 3.1196 -0.0936 -0.6467
C 3.3102 1.0823 -1.4146
C 4.3437 1.0777 -2.3666
C 5.1378 -0.0554 -2.5684
C 4.8974 -1.2176 -1.8312
C 3.8819 -1.2687 -0.8606
H 4.5223 1.9665 -2.9610
H 5.9307 -0.0367 -3.3089
H 5.5000 -2.1013 -2.0133
C 0.2641 -1.0054 -1.9920
H 1.3366 -0.9332 -2.1875
H -0.0612 -2.0409 -2.1487
C -0.5315 -0.0304 -2.8534
H -1.6040 -0.1303 -2.6510
H -0.2639 1.0021 -2.6005
C -0.2767 -0.2635 -4.3547
H 0.7819 -0.1280 -4.6015
H -0.5585 -1.2803 -4.6498
H -0.8576 0.4377 -4.9631
C 4.8984 0.7466 1.9275
C 3.5735 0.5381 2.2954
C 3.2011 0.7075 3.6651
C 4.1159 1.0760 4.6747
C 5.4672 1.2820 4.2650
C 5.8335 1.1198 2.9326
H 5.2297 0.6313 0.9038
C 1.8185 0.4661 3.9197
C 3.5901 1.2013 5.9961
H 6.2125 1.5666 5.0011
H 6.8659 1.2813 2.6428
C 2.2421 0.9661 6.2460
C 1.3336 0.5950 5.2147
H 4.2511 1.4824 6.8099
H 1.8644 1.0667 7.2575
H 0.2911 0.4208 5.4512
C 0.1724 -3.3145 4.6482
C -0.5823 -2.8631 3.3733
H 0.8146 -2.5156 5.0353
H -0.5320 -3.5947 5.4405
H 0.8017 -4.1858 4.4321
C -1.4279 -4.0233 2.7981
H 0.1693 -2.6082 2.6167
H -1.9448 -3.7167 1.8816
H -0.7835 -4.8765 2.5566
H -2.1814 -4.3698 3.5146
C -2.6395 2.5445 1.6471
C -1.5621 2.1598 2.6913
H -2.7226 1.7778 0.8680
H -3.6228 2.6603 2.1180
H -2.3819 3.4952 1.1660
C -1.3945 3.2758 3.7491
H -0.6111 2.0727 2.1541
H -0.6095 3.0245 4.4708
H -1.1223 4.2198 3.2633
H -2.3242 3.4440 4.3048
C 3.1391 -3.6872 -1.0721
C 3.6222 -2.5765 -0.1068
H 2.2351 -3.3797 -1.6087
H 3.9077 -3.9293 -1.8150
H 2.9131 -4.6025 -0.5125
C 4.8663 -3.0430 0.6868
H 2.8157 -2.4050 0.6149
H 5.1975 -2.2786 1.3980
H 4.6362 -3.9561 1.2480
H 5.7040 -3.2670 0.0161
C 3.1227 3.3727 -0.3074
C 2.4357 2.3255 -1.2210
H 3.3574 2.9614 0.6796
H 4.0598 3.7199 -0.7592
H 2.4708 4.2434 -0.1696
C 2.0303 2.9789 -2.5625
H 1.5114 2.0037 -0.7224
H 1.6015 2.2465 -3.2539
H 1.2845 3.7622 -2.3845
H 2.8858 3.4516 -3.0581
N -1.8862 -1.2484 -0.1733
C -2.9925 -1.5760 -0.2488
C -4.3675 -1.9929 -0.3341
H -4.8314 -2.0032 0.6665
H -4.4505 -2.9973 -0.7652
H -4.9472 -1.2971 -0.9675

[Pd](CH3CN)CH(CH3)2+
598 -1883.056738
Pd -0.0237 0.0011 -0.0384
N -0.0092 -0.0247 2.2252
N 2.0605 -0.0427 0.3982
C 1.1942 -0.0456 2.6734
C 2.3337 -0.0577 1.6658
C -1.1662 -0.0015 3.0860
C -1.8280 -1.2234 3.3667
C -2.9922 -1.1747 4.1520
C -3.4978 0.0404 4.6240
C -2.8462 1.2356 4.3066
C -1.6737 1.2449 3.5311
H -3.5050 -2.0992 4.3974
H -4.3959 0.0559 5.2332
H -3.2503 2.1768 4.6654
C 3.1427 -0.0902 -0.5680
C 3.6144 1.1286 -1.1209
C 4.6836 1.0612 -2.0297
C 5.2467 -0.1656 -2.3945
C 4.7294 -1.3547 -1.8744
C 3.6612 -1.3488 -0.9604
H 5.0740 1.9760 -2.4608
H 6.0750 -0.1949 -3.0949
H 5.1534 -2.3034 -2.1859
C 0.1910 0.0118 -2.0977
H 1.2785 -0.0351 -2.2072
C -0.4525 -1.2282 -2.7052
C -0.3457 1.3136 -2.6795
H -1.4353 1.3792 -2.5991
H 0.0846 2.1950 -2.1968
H -0.0949 1.3715 -3.7499
H -0.1865 -1.2996 -3.7709
H -1.5448 -1.1935 -2.6467
H -0.1170 -2.1519 -2.2244
C 4.9433 -0.0843 2.1159
C 3.5893 -0.0820 2.4349
C 3.2060 -0.0911 3.8120
C 4.1355 -0.1139 4.8745
C 5.5157 -0.1190 4.5130
C 5.8939 -0.1017 3.1744
H 5.2867 -0.0737 1.0900
C 1.7950 -0.0722 4.0158
C 3.5942 -0.1272 6.1956
H 6.2732 -0.1353 5.2904
H 6.9484 -0.1032 2.9211
C 2.2179 -0.1148 6.3955
C 1.2952 -0.0847 5.3117
H 4.2657 -0.1467 7.0483
H 1.8283 -0.1263 7.4076
H 0.2308 -0.0713 5.5106
C -0.7303 -3.4257 4.0125
C -1.3022 -2.5679 2.8566
H 0.0729 -2.8992 4.5401
H -1.5112 -3.6682 4.7432
H -0.3258 -4.3683 3.6257
C -2.3825 -3.3518 2.0753
H -0.4826 -2.3657 2.1569
H -2.7696 -2.7604 1.2376
H -1.9585 -4.2783 1.6712
H -3.2268 -3.6266 2.7179
C -1.9353 3.4270 2.2609
C -1.0127 2.5781 3.1699
H -2.1927 2.8826 1.3449
H -2.8670 3.6885 2.7762
H -1.4357 4.3602 1.9755
C -0.5917 3.3758 4.4268
H -0.1035 2.3663 2.5964
H 0.0881 2.7931 5.0581
H -0.0794 4.3000 4.1354
H -1.4615 3.6542 5.0330
C 2.6535 -3.5912 -1.6186
C 3.0929 -2.6773 -0.4493
H 1.9573 -3.0766 -2.2883
H 3.5131 -3.9188 -2.2140
H 2.1588 -4.4885 -1.2288
C 4.0949 -3.4261 0.4650
H 2.1971 -2.4587 0.1445
H 4.3819 -2.8223 1.3315
H 3.6496 -4.3588 0.8305
H 5.0079 -3.6843 -0.0847
C 3.7884 3.1745 0.3951
C 2.9964 2.4790 -0.7417
H 3.8378 2.5560 1.2968
H 4.8160 3.3840 0.0741
H 3.3154 4.1277 0.6593
C 2.8653 3.4330 -1.9509
H 1.9824 2.2819 -0.3671
H 2.3729 2.9451 -2.7981
H 2.2740 4.3117 -1.6686
H 3.8424 3.7955 -2.2895
N -2.0598 0.0631 -0.2522
C -3.2154 0.0968 -0.2711
C -4.6722 0.1349 -0.2808
H -5.0473 0.0625 0.7451
H -5.0637 -0.7031 -0.8664
H -5.0191 1.0737 -0.7243

[Pd]{S(CH3)2}CH3+
568 -2149.710295
Pd -0.0568 0.0557 0.0161
N 0.0145 -0.0255 2.2679
N 2.0368 -0.0010 0.3934
C 1.2335 -0.0707 2.6823
C 2.3455 -0.0693 1.6482
C -1.1011 0.0489 3.1793
C -1.8743 -1.1222 3.3818
C -2.9937 -1.0346 4.2233
C -3.3515 0.1769 4.8233
C -2.5931 1.3255 4.5844
C -1.4545 1.2936 3.7596
H -3.5934 -1.9192 4.4067
H -4.2227 0.2264 5.4681
H -2.8881 2.2644 5.0412
C 3.0753 -0.0131 -0.6189
C 3.5554 1.2240 -1.1157
C 4.5582 1.1873 -2.0997
C 5.0492 -0.0267 -2.5880
C 4.5299 -1.2331 -2.1100
C 3.5274 -1.2569 -1.1252
H 4.9530 2.1195 -2.4898
H 5.8248 -0.0326 -3.3469
H 4.9017 -2.1707 -2.5099
C 0.1407 0.1626 -2.0117
H 1.1582 0.4867 -2.2289
H -0.0262 -0.8399 -2.4194
H -0.5770 0.8674 -2.4395
C 4.9639 -0.1594 2.0142
C 3.6212 -0.1364 2.3761
C 3.2766 -0.1801 3.7618
C 4.2365 -0.2597 4.7938
C 5.6052 -0.2816 4.3905
C 5.9449 -0.2301 3.0423
H 5.2750 -0.1275 0.9782
C 1.8715 -0.1414 4.0065
C 3.7341 -0.3117 6.1289
H 6.3845 -0.3394 5.1439
H 6.9912 -0.2467 2.7578
C 2.3644 -0.2856 6.3694
C 1.4110 -0.1986 5.3160
H 4.4295 -0.3738 6.9601
H 2.0040 -0.3303 7.3912
H 0.3537 -0.1765 5.5481
C -0.6158 -3.3067 3.7067
C -1.4738 -2.4517 2.7388
H 0.2840 -2.7720 4.0296
H -1.1931 -3.5664 4.6022
H -0.3045 -4.2391 3.2209
C -2.6846 -3.2659 2.2323
H -0.8479 -2.2178 1.8658
H -3.3310 -2.6628 1.5844
H -2.3371 -4.1367 1.6641
H -3.2965 -3.6430 3.0595
C -1.5306 3.5823 2.6604
C -0.6818 2.5898 3.4923
H -1.8244 3.1408 1.7010
H -2.4441 3.8667 3.1949
H -0.9594 4.4951 2.4551
C -0.1923 3.2596 4.7981
H 0.2056 2.3496 2.8967
H 0.4315 2.5790 5.3869
H 0.4018 4.1506 4.5646
H -1.0338 3.5766 5.4244
C 2.2940 -3.3670 -1.8242
C 2.9577 -2.5986 -0.6556
H 1.5118 -2.7652 -2.3001
H 3.0272 -3.6350 -2.5933
H 1.8411 -4.2953 -1.4569
C 4.0361 -3.4733 0.0297
H 2.1740 -2.3984 0.0840
H 4.4862 -2.9583 0.8852
H 3.5935 -4.4098 0.3884
H 4.8393 -3.7300 -0.6710
C 4.0887 3.3309 0.2117
C 3.0221 2.5693 -0.6145
H 4.4318 2.7396 1.0677
H 4.9629 3.5698 -0.4055
H 3.6762 4.2737 0.5894
C 2.5013 3.4502 -1.7749
H 2.1697 2.3693 0.0462
H 1.7345 2.9284 -2.3576
H 2.0628 4.3730 -1.3777
H 3.3092 3.7354 -2.4581
S -2.4267 0.0145 -0.1770
C -2.9986 1.5794 -0.9234
H -4.0845 1.5326 -1.0395
H -2.7424 2.3814 -0.2289
H -2.5199 1.7569 -1.8885
C -2.9184 -1.1532 -1.4900
H -2.4378 -0.9075 -2.4386
H -2.6129 -2.1499 -1.1657
H -4.0061 -1.1219 -1.5921

[Pd]{S(CH3)2}CH2CH2CH3+
616 -2228.338456
Pd -0.0503 -0.0574 0.0053
N 0.0071 -0.0553 2.2729
N 2.0576 -0.0136 0.4180
C 1.2211 -0.0808 2.6995
C 2.3461 -0.0949 1.6768
C -1.1213 0.0686 3.1649
C -1.8864 -1.0903 3.4587
C -3.0266 -0.9362 4.2648
C -3.4088 0.3193 4.7472
C -2.6540 1.4500 4.4261
C -1.4971 1.3569 3.6313
H -3.6228 -1.8063 4.5144
H -4.2945 0.4160 5.3668
H -2.9626 2.4217 4.7981
C 3.1162 -0.0350 -0.5716
C 3.6142 1.1984 -1.0619
C 4.6408 1.1522 -2.0199
C 5.1371 -0.0672 -2.4914
C 4.5982 -1.2689 -2.0240
C 3.5737 -1.2832 -1.0616
H 5.0493 2.0793 -2.4063
H 5.9306 -0.0797 -3.2315
H 4.9710 -2.2103 -2.4141
C 0.1712 0.1204 -2.0290
H 1.2459 0.0110 -2.1940
H -0.3386 -0.7205 -2.5106
C -0.3295 1.4622 -2.5548
H -1.4048 1.5787 -2.3677
H 0.1629 2.2826 -2.0199
C -0.0706 1.6198 -4.0661
H 0.9996 1.5555 -4.2897
H -0.5753 0.8329 -4.6376
H -0.4348 2.5870 -4.4280
C 4.9573 -0.2446 2.0788
C 3.6115 -0.1804 2.4230
C 3.2507 -0.1840 3.8054
C 4.1966 -0.2556 4.8510
C 5.5688 -0.3222 4.4649
C 5.9244 -0.3157 3.1201
H 5.2816 -0.2416 1.0463
C 1.8444 -0.1124 4.0325
C 3.6783 -0.2559 6.1810
H 6.3378 -0.3790 5.2290
H 6.9730 -0.3667 2.8484
C 2.3071 -0.1897 6.4047
C 1.3680 -0.1176 5.3376
H 4.3628 -0.3094 7.0218
H 1.9344 -0.1932 7.4231
H 0.3086 -0.0690 5.5562
C -0.5888 -3.2122 4.0012
C -1.4616 -2.4725 2.9537
H 0.3077 -2.6404 4.2618
H -1.1590 -3.3847 4.9221
H -0.2713 -4.1867 3.6117
C -2.6546 -3.3613 2.5392
H -0.8426 -2.3172 2.0595
H -3.3151 -2.8425 1.8368
H -2.2860 -4.2733 2.0558
H -3.2501 -3.6730 3.4049
C -1.5534 3.6148 2.4476
C -0.7124 2.6320 3.2986
H -1.8562 3.1619 1.4970
H -2.4590 3.9285 2.9795
H -0.9697 4.5147 2.2213
C -0.1961 3.3367 4.5771
H 0.1615 2.3560 2.6985
H 0.4262 2.6676 5.1800
H 0.4056 4.2126 4.3083
H -1.0271 3.6824 5.2027
C 2.2864 -3.3486 -1.7863
C 2.9772 -2.6191 -0.6076
H 1.5074 -2.7232 -2.2363
H 3.0073 -3.6068 -2.5705
H 1.8236 -4.2788 -1.4360
C 4.0359 -3.5320 0.0561
H 2.2039 -2.4135 0.1412
H 4.5068 -3.0403 0.9142
H 3.5684 -4.4590 0.4077
H 4.8257 -3.8057 -0.6530
C 3.9603 3.1483 0.5448
C 3.0686 2.5417 -0.5690
H 4.0523 2.4771 1.4048
H 4.9692 3.3461 0.1628
H 3.5386 4.0981 0.8942
C 2.8866 3.5638 -1.7147
H 2.0769 2.3543 -0.1356
H 2.3091 3.1426 -2.5441
H 2.3593 4.4497 -1.3427
H 3.8503 3.9026 -2.1116
S -2.3790 -0.5575 -0.1755
C -3.3491 0.9761 0.0152
H -4.4089 0.7363 -0.1072
H -3.1767 1.3361 1.0306
H -3.0435 1.7329 -0.7105
C -2.9091 -1.0625 -1.8451
H -2.6629 -0.3065 -2.5933
H -2.4002 -1.9995 -2.0797
H -3.9885 -1.2343 -1.8219

[Pd]{S(CH3)2}CH(CH3)2+
616 -2228.333674
Pd -0.0602 -0.1218 -0.0470
N -0.0582 -0.0505 2.2945
N 2.0527 -0.1132 0.4847
C 1.1474 -0.0951 2.7427
C 2.3008 -0.0785 1.7533
C -1.1713 -0.1248 3.2115
C -1.6409 -1.3965 3.6292
C -2.7455 -1.4313 4.4991
C -3.3669 -0.2575 4.9332
C -2.9046 0.9845 4.4847
C -1.8091 1.0797 3.6096
H -3.1210 -2.3910 4.8387
H -4.2137 -0.3089 5.6098
H -3.4031 1.8887 4.8153
C 3.1625 -0.0620 -0.4484
C 3.6182 1.2040 -0.8968
C 4.7203 1.2276 -1.7681
C 5.3308 0.0451 -2.1967
C 4.8269 -1.1920 -1.7845
C 3.7265 -1.2766 -0.9141
H 5.1003 2.1814 -2.1176
H 6.1851 0.0873 -2.8644
H 5.2874 -2.1039 -2.1481
C 0.3364 -0.4942 -2.0600
H 1.4255 -0.5490 -2.0068
C -0.2452 -1.8516 -2.4352
C -0.0633 0.6193 -3.0180
H -1.1463 0.6756 -3.1718
H 0.3017 1.5979 -2.6923
H 0.3804 0.4223 -4.0053
H 0.1422 -2.1567 -3.4192
H -1.3366 -1.8262 -2.5148
H 0.0323 -2.6333 -1.7218
C 4.9044 -0.0069 2.2360
C 3.5476 -0.0516 2.5390
C 3.1488 -0.1019 3.9093
C 4.0671 -0.1082 4.9822
C 5.4507 -0.0619 4.6378
C 5.8435 -0.0123 3.3046
H 5.2595 0.0317 1.2148
C 1.7355 -0.1420 4.0944
C 3.5134 -0.1585 6.2966
H 6.1987 -0.0648 5.4245
H 6.9001 0.0234 3.0634
C 2.1356 -0.1963 6.4802
C 1.2251 -0.1874 5.3865
H 4.1761 -0.1666 7.1563
H 1.7344 -0.2338 7.4870
H 0.1602 -0.2163 5.5774
C -0.3926 -3.4999 4.3567
C -0.9998 -2.7114 3.1701
H 0.3525 -2.9052 4.8948
H -1.1691 -3.7975 5.0712
H 0.0949 -4.4123 3.9943
C -2.0039 -3.5985 2.3947
H -0.1844 -2.4723 2.4782
H -2.3904 -3.0834 1.5082
H -1.5142 -4.5208 2.0615
H -2.8571 -3.8810 3.0218
C -2.4664 3.4403 2.8505
C -1.3143 2.4445 3.1183
H -3.2561 2.9996 2.2316
H -2.9283 3.7819 3.7836
H -2.0806 4.3291 2.3383
C -0.2991 3.0809 4.1028
H -0.7884 2.2754 2.1674
H 0.5753 2.4426 4.2579
H 0.0466 4.0483 3.7195
H -0.7697 3.2515 5.0786
C 3.0117 -3.5970 -1.7080
C 3.1713 -2.6440 -0.5002
H 2.4439 -3.1292 -2.5184
H 3.9835 -3.9055 -2.1095
H 2.4834 -4.5061 -1.3986
C 4.0393 -3.3176 0.5929
H 2.1713 -2.4804 -0.0771
H 4.1144 -2.6998 1.4930
H 3.6080 -4.2850 0.8759
H 5.0553 -3.4974 0.2211
C 3.7961 3.2701 0.5963
C 2.9530 2.5148 -0.4620
H 3.9639 2.6638 1.4918
H 4.7756 3.5441 0.1860
H 3.2876 4.1935 0.8980
C 2.6569 3.4428 -1.6638
H 1.9886 2.2621 -0.0028
H 2.0951 2.9208 -2.4454
H 2.0686 4.3066 -1.3327
H 3.5787 3.8284 -2.1138
S -2.3605 0.1601 -0.7238
C -2.5981 1.9708 -0.7945
H -2.3517 2.4354 0.1609
H -1.9387 2.3550 -1.5742
H -3.6375 2.1786 -1.0634
C -3.5407 -0.2469 0.6070
H -4.5427 0.0254 0.2639
H -3.4961 -1.3255 0.7647
H -3.2987 0.2699 1.5358