

## SUPPORTING INFORMATION

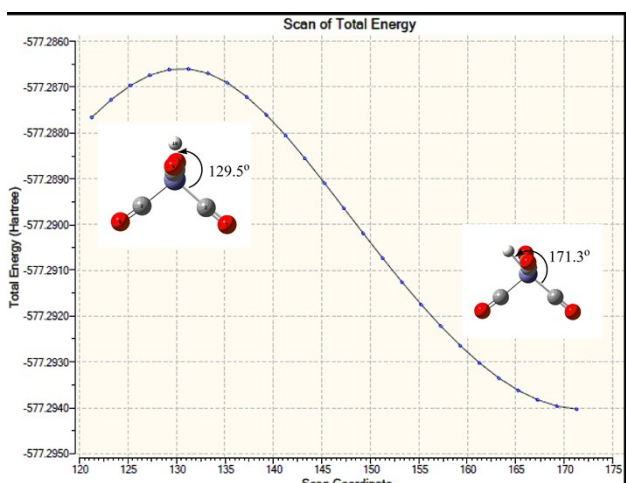
### Revisiting the Polytopal Rearrangements in Penta-Coordinate d7-Metallocomplexes: Modified Berry Pseudorotation, Octahedral Switch, and Butterfly Isomerization

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Figure S1. Direct relaxed scan of the C-Fe\_H angle from the qSP equilibrium state leading to TS<sub>OSH</sub>.



(see text, Sec. 3.4, Butterfly Isomerization.).

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Full Citation for Ref. [72]

Gaussian 03, Revision D.01,  
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J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

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**Table S1.** Geometries and  
Frequencies of HFe(CO)<sub>4</sub> Radical  
Calculated at Different Levels  
Presented in Table 1.

UBP86/LanL2TZ(f) ECP[Fe]/  
aug-cc-pVDZ [C,O,H] (BS-I)

*Quasi-SP*

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

|    |           |           |           |
|----|-----------|-----------|-----------|
| 26 | 0.000008  | -0.025568 | -0.305942 |
| 6  | -0.000030 | 1.558936  | 0.579702  |
| 6  | 0.000013  | -1.117223 | 1.121329  |
| 6  | 1.742169  | -0.151678 | -0.759653 |
| 6  | -1.742146 | -0.151723 | -0.759671 |
| 8  | 2.847913  | -0.303200 | -1.080997 |
| 8  | -0.000080 | 2.572699  | 1.147131  |
| 8  | 0.000015  | -1.836956 | 2.034184  |
| 8  | -2.847880 | -0.303284 | -1.081033 |
| 1  | 0.000028  | -1.199183 | -1.290039 |

*Frequencies, cm<sup>-1</sup>*

|          |          |          |
|----------|----------|----------|
| 68.4396  | 79.6159  | 88.4631  |
| 92.9108  | 98.7021  | 308.3970 |
| 350.7729 | 356.0121 | 425.5139 |
| 445.8352 | 474.4454 | 478.6935 |
| 491.4346 | 518.5554 | 527.5544 |

558.6573 594.7186 677.8909  
705.6592 1886.1504 1981.8608  
1984.0827 1993.8076 2057.0068

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**EBT**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.000003 -0.000001 -0.030909  
6 -0.008716 -1.727252 0.426397  
6 0.008707 1.727274 0.426310  
6 -1.758043 0.008984 -0.503837  
6 1.758059 -0.009012 -0.503795  
8 -2.879878 0.015040 -0.807403  
8 -0.014242 -2.820526 0.823519  
8 0.014226 2.820566 0.823380  
8 2.879883 -0.015080 -0.807405  
1 -0.000027 0.000043 1.476448

*Frequencies, cm<sup>-1</sup>*

54.7063 87.4244 89.9554  
91.9589 105.0148 329.7259  
371.8623 387.6874 415.7155  
458.3961 483.1697 485.2348  
490.2882 523.7436 551.6471  
583.1640 616.9070 638.9542  
681.2923 1915.0712 1965.0095  
1980.2404 1983.8952 2058.4764

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**TS<sub>mBPR</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.000005 -0.000013 -0.032881  
6 -0.575347 -1.708435 -0.039583  
6 0.575327 1.708420 -0.039602  
6 -1.708417 0.575341 -0.039566  
6 1.708438 -0.575334 -0.039626  
8 -2.808722 0.945960 0.010693  
8 -0.945965 -2.808741 0.010665  
8 0.945905 2.808740 0.010629  
8 2.808759 -0.945910 0.010590  
1 0.000032 -0.000016 1.464539

*Frequencies, cm<sup>-1</sup>*

-60.4432 92.5324 92.5329  
96.6569 107.3061 350.9530  
353.5384 353.5390 384.6951  
447.0413 460.4196 484.9736  
484.9751 561.7865 623.0380  
623.0390 652.0539 734.9852

734.9866 1914.5365 1974.3881  
1974.3930 1994.0426 2071.2594

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**TS<sub>OSH</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.000012 -0.000003 -0.331401  
6 -0.000007 1.359326 0.860733  
6 -0.000007 -1.359311 0.860757  
6 1.751608 -0.000007 -0.733459  
6 -1.751578 -0.000007 -0.733483  
8 2.872339 -0.000009 -1.036806  
8 -0.000043 2.258681 1.597840  
8 -0.000043 -2.258652 1.597881  
8 -2.872306 -0.000009 -1.036844  
1 0.000023 -0.000017 -1.887433

*Frequencies, cm<sup>-1</sup>*

-490.8764 73.6951 79.4567  
85.5812 95.0300 105.4588  
317.8389 354.4739 364.0252  
435.2951 450.1805 454.4935  
485.5580 515.9610 535.9780  
542.6469 562.1139 610.0055  
664.3102 1827.1296 1973.2892  
1986.2363 1989.4727 2058.0897

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**TS<sub>OSL</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.132630 0.000359 -0.144593  
6 -0.058038 -0.004449 1.659401  
6 -0.965951 1.360206 -0.516274  
6 -0.966771 -1.356815 -0.523547  
6 1.960354 0.000518 -0.410575  
8 -1.655690 -2.250352 -0.807539  
8 -0.217860 -0.007520 2.810123  
8 -1.654341 2.255656 -0.795481  
8 3.086386 0.000902 -0.686033  
1 0.266085 0.004408 -1.663160

*Frequencies, cm<sup>-1</sup>*

-337.4393 72.7162 75.4490  
93.0402 96.8229 141.6722  
326.8808 333.9619 338.3500  
410.8621 462.1880 482.2489  
499.2472 525.2955 536.1859  
554.3941 587.7086 661.8092  
719.5485 1900.8645 1971.0948

1989.2327 1992.9728 2050.1103

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**TS<sub>BFI</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000620 0.027481 -0.086659  
6 -0.038918 1.749694 0.623871  
6 0.035601 -1.583360 0.700312  
6 1.717701 -0.017899 -0.576265  
6 -1.715500 -0.094619 -0.575197  
8 2.804423 -0.083113 -0.986732  
8 -0.062816 2.820635 1.066443  
8 0.058688 -2.610040 1.249482  
8 -2.798476 -0.208333 -0.984993  
1 0.008258 -0.390587 -1.536783

*Frequencies, cm<sup>-1</sup>*

-421.1243 72.6195 75.0622  
89.5681 92.7034 119.2074  
316.9151 358.0102 379.5419  
408.0109 465.7871 468.5998  
494.2993 517.1361 536.0585  
552.5862 572.9303 628.1067  
676.0283 1930.6426 1965.9173  
1978.2932 1989.3040 2051.8197

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**UB3LYP/ LanL2TZ(f) ECP[Fe]/  
aug-cc-pVDZ [C,O,H] (BS-I)**  
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**Quasi-SP**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.000082 0.002786 -0.306823  
6 -0.000970 1.487272 0.764963  
6 0.000481 -1.294636 0.994261  
6 1.764069 -0.036078 -0.765276  
6 -1.763676 -0.037891 -0.766003  
8 2.856903 -0.120792 -1.099123  
8 -0.001669 2.418534 1.433838  
8 0.000761 -2.139954 1.768376  
8 -2.856302 -0.123691 -1.100250  
1 0.000899 -1.057206 -1.412986

*Frequencies, cm<sup>-1</sup>*

66.6773 80.6032 91.4446  
95.0798 101.2368 297.4292  
345.8129 357.7503 399.8700  
419.6640 451.5214 460.6365

480.8571 516.7320 536.7642  
580.4519 589.5223 674.8022  
754.1921 1879.5253 2068.7308  
2070.2919 2076.3309 2145.7802

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**EBT**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000004 0.000006 -0.024849  
6 -0.009119 -1.752902 0.395394  
6 0.009107 1.752935 0.395306  
6 -1.786819 0.009125 -0.480128  
6 1.786813 -0.009143 -0.480112  
8 -2.900163 0.014534 -0.752124  
8 -0.014808 -2.841685 0.758348  
8 0.014796 2.841734 0.758212  
8 2.900162 -0.014577 -0.752091  
1 -0.000003 0.000050 1.492576

*Frequencies, cm<sup>-1</sup>*

48.8331 91.5756 93.1941  
96.3287 109.8384 328.2855  
367.1826 386.3228 392.0007  
437.8910 459.7552 472.7786  
476.1667 538.3400 562.5344  
591.2840 620.5324 668.6479  
668.9916 1842.4342 2054.5324  
2064.7381 2070.0468 2144.5907

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**TS<sub>mBPR</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.000000 0.000003 -0.041346  
6 1.784361 -0.370619 -0.042503  
6 -1.784364 0.370613 -0.042523  
6 -0.370614 -1.784360 -0.042481  
6 0.370618 1.784365 -0.042546  
8 -0.603731 -2.905162 0.019678  
8 2.905163 -0.603744 0.019642  
8 -2.905169 0.603723 0.019614  
8 0.603736 2.905169 0.019576  
1 -0.000004 0.000033 1.467228

*Frequencies, cm<sup>-1</sup>*

-50.6625 97.9280 97.9281  
99.9413 112.7273 356.5036  
358.4912 358.4987 379.3526  
415.7437 436.9549 466.0367  
466.0379 575.8323 629.0189

629.0191 648.8352 730.9759  
730.9842 1822.6459 2062.3193  
2062.3221 2072.3614 2152.2074

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**TS<sub>OSH</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000010 -0.000003 0.340414  
6 0.000010 1.415029 -0.843960  
6 0.000010 -1.415013 -0.843986  
6 -1.776711 -0.000006 0.698687  
6 1.776683 -0.000006 0.698724  
8 -2.889184 -0.000008 0.971759  
8 0.000039 2.330549 -1.534443  
8 0.000039 -2.330522 -1.534485  
8 2.889150 -0.000008 0.971819  
1 -0.000024 -0.000018 1.895220

*Frequencies, cm<sup>-1</sup>*

-444.6437 71.3226 81.5131  
86.8718 96.6779 107.7689  
305.1212 360.0314 360.4394  
400.8993 432.1787 450.1363  
457.3949 520.9123 527.0728  
557.0092 576.6546 608.1596  
691.8571 1819.2074 2060.1161  
2073.8790 2078.1372 2147.7161

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**TS<sub>OSL</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.122243 0.000389 -0.154294  
6 0.060395 -0.004467 1.665359  
6 0.976544 1.399424 -0.512176  
6 0.977386 -1.396048 -0.519646  
6 1.977762 0.000495 -0.403129  
8 1.640336 -2.288415 -0.804487  
8 0.209588 -0.007513 2.802169  
8 1.638958 2.293697 -0.792246  
8 3.089779 0.000858 -0.667492  
1 0.233899 0.004424 -1.674358

*Frequencies, cm<sup>-1</sup>*

-334.9497 71.9204 77.2034  
94.1364 99.6727 138.8327  
331.9160 332.9063 335.8538  
383.2371 447.6260 452.3913  
553.5479 588.3244 706.4226  
764.8597 1896.8097 2055.8841

2069.7666 2085.2395 2141.7611

-----  
**TS<sub>BFI</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000785 0.022654 -0.087917  
6 -0.039718 1.783379 0.599976  
6 0.036536 -1.623565 0.698107  
6 1.738064 -0.016396 -0.555915  
6 -1.736401 -0.094097 -0.555052  
8 2.816978 -0.072887 -0.944713  
8 -0.063056 2.848935 1.013118  
8 0.059888 -2.647494 1.216330  
8 -2.811910 -0.198713 -0.943300  
1 0.007456 -0.345070 -1.558931

*Frequencies, cm<sup>-1</sup>*

-422.4329 70.6733 78.2627  
92.7032 97.2579 121.5168  
308.8870 354.7663 377.6276  
383.6198 450.2207 465.2286  
467.7932 503.2989 543.7080  
571.1000 575.4699 653.3038  
658.6135 1879.0579 2053.5229  
2062.0476 2078.5862 2141.2651

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**UB3LYP/ 6-311+G(2d,p) (BS-II)**  
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**Quasi-SP**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.023876 -0.290159 -0.012445  
6 1.383987 0.909462 -0.010109  
6 -1.423765 0.911196 -0.002879  
6 -0.015964 -0.761963 1.760922  
6 -0.024697 -0.744970 -1.789825  
8 0.051083 -1.105815 2.843343  
8 2.286688 1.602727 -0.008997  
8 -2.289250 1.650704 0.002273  
8 0.037089 -1.078873 -2.875719  
1 0.961575 -1.465256 -0.021688

*Frequencies, cm<sup>-1</sup>*

64.6841 77.7144 87.1066  
90.0485 95.7063 284.4441  
337.0082 347.3547 390.0192  
408.3873 440.3727 447.8220

473.8726 503.9525 526.6561  
747.1709 1892.7817 2085.0780  
2085.8560 2091.7722 2160.5007

-----  
**EBT**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000065 -0.252835 0.000000  
6 1.797686 0.211012 0.000000  
6 -1.797676 0.211534 0.000000  
6 -0.000129 -0.685203 1.759352  
6 -0.000129 -0.685203 -1.759352  
8 -0.000185 -1.058009 2.836524  
8 2.903746 0.479217 0.000000  
8 -2.903656 0.480065 0.000000  
8 -0.000185 -1.058009 -2.836524  
1 -0.000293 -1.776526 0.000000

*Frequencies, cm<sup>-1</sup>*

46.4058 86.9424 89.9798  
92.0391 105.6183 318.5296  
357.9022 375.2853 388.6423  
424.3720 454.2967 465.4233  
465.7808 516.0613 553.0133  
580.4839 606.1385 654.9091  
662.1264 1833.7176 2071.2977  
2078.5412 2084.1434 2157.5741

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**TS<sub>mBPR</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000095 -0.334111 0.000000  
6 1.831180 -0.339759 0.000000  
6 -1.831374 -0.339195 0.000000  
6 -0.000088 -0.339386 1.831269  
6 -0.000088 -0.339386 -1.831269  
8 -0.000092 -0.413291 2.967362  
8 2.967262 -0.413831 0.000000  
8 -2.967478 -0.412912 0.000000  
8 -0.000092 -0.413291 -2.967362  
1 -0.000328 -1.852440 0.000000

*Frequencies, cm<sup>-1</sup>*

-48.3320 94.3169 94.3233  
96.7717 108.6290 345.8954  
353.4360 353.4419 370.5155  
410.9913 432.2864 460.1767  
460.1899 567.4932 621.8980  
621.9000 634.1539 717.4076

717.4198 1791.0908 2078.0191  
2078.0194 2088.0973 2166.1564

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**TS<sub>OSH</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000086 -0.345380 0.000000  
6 1.421032 0.851397 0.000000  
6 -1.420831 0.851842 0.000000  
6 -0.000141 -0.705194 1.786937  
6 -0.000141 -0.705194 -1.786937  
8 -0.000184 -0.976543 2.891611  
8 2.330959 1.535856 0.000000  
8 -2.330547 1.536580 0.000000  
8 -0.000184 -0.976543 -2.891611  
1 -0.000337 -1.905576 0.000000

*Frequencies, cm<sup>-1</sup>*

-443.8016 70.2927 79.0364  
83.6499 92.2336 103.1009  
306.6370 351.1147 352.7344  
390.4547 421.7413 437.2125  
448.4587 511.3222 515.5509  
548.3676 564.0527 595.9056  
687.0361 1824.9193 2076.2812  
2089.3352 2093.6070 2162.2411

-----  
**TS<sub>OSL</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.124106 0.000382 -0.154618  
6 -0.059721 -0.004505 1.678047  
6 -0.985617 1.404469 -0.513552  
6 -0.986461 -1.401087 -0.521077  
6 1.996879 0.000485 -0.402562  
8 -1.647878 -2.283527 -0.808671  
8 -0.211335 -0.007486 2.806425  
8 -1.646504 2.288832 -0.796415  
8 3.099735 0.000865 -0.669911  
1 0.230612 0.004418 -1.676500

*Frequencies, cm<sup>-1</sup>*

-298.6011 71.0431 75.6804  
91.1203 95.2060 136.4060  
325.9076 327.7245 329.0537  
373.3945 438.6189 441.2246  
460.8494 510.8859 543.5615  
545.4262 575.8688 710.0587  
766.1374 1915.5012 2070.5022

2084.6289 2102.3050 2156.9443

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**TS<sub>BFI</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.000052 0.024458 -0.081978  
6 0.000207 1.800979 0.610306  
6 0.000134 -1.636062 0.702373  
6 1.745368 -0.054657 -0.558048  
6 -1.745424 -0.054567 -0.557471  
8 2.811841 -0.138847 -0.952724  
8 0.000288 2.860203 1.017827  
8 0.000176 -2.657026 1.209285  
8 -2.812031 -0.138702 -0.951794  
1 -0.000205 -0.345059 -1.557656

*Frequencies, cm<sup>-1</sup>*

-401.9689 69.2474 76.1941  
89.6379 93.8461 115.7948  
297.0127 347.2106 367.3692  
380.6853 440.8454 457.8011  
460.7885 495.2782 534.5544  
561.8362 567.5326 647.1821  
659.4143 1878.9720 2067.8493  
2076.3958 2095.5005 2155.6685

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**UMP2/ LanL2TZ(f) ECP[Fe]/  
aug-cc-pVDZ [C,O,H] (BS-I)**  
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**Quasi-SP**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.000000 -0.065507 -0.321489  
6 0.000011 1.485459 0.441602  
6 -0.000011 -0.939180 1.114182  
6 1.657447 -0.235040 -0.744201  
6 -1.657446 -0.235013 -0.744212  
8 2.788708 -0.365988 -0.978603  
8 0.000018 2.534018 0.952633  
8 -0.000018 -1.496443 2.144812  
8 -2.788708 -0.365942 -0.978621  
1 -0.000006 -1.208363 -1.113024

*Frequencies, cm<sup>-1</sup>*

86.3222 100.7886 107.8092  
109.8086 115.2651 405.0044  
470.8867 496.4196 519.2793  
565.9236 569.4428 626.7223

634.8723 664.2465 695.0544  
752.1245 821.6941 895.0807  
1165.5376 2012.0757 2036.6218  
2062.2964 2150.5737 2560.0536  
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**EBT**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.000015 -0.000174 0.005477  
6 0.110082 -1.570059 0.618652  
6 -0.110093 1.570099 0.617986  
6 -1.597211 -0.111720 -0.648747  
6 1.597219 0.111822 -0.648721  
8 -2.662627 -0.186052 -1.123358  
8 0.185581 -2.645801 1.048785  
8 -0.185600 2.645806 1.048385  
8 2.662599 0.186627 -1.123337  
1 0.000037 -0.000516 1.358988

*Frequencies, cm<sup>-1</sup>*

95.6748 98.6789 99.5561  
108.8520 139.7546 353.2056  
439.2769 454.8167 505.7318  
545.3488 565.1078 569.5012  
630.0876 654.9483 740.1582  
751.9260 846.3033 885.0426  
1166.0647 1996.7652 2020.7196  
2148.9099 2317.7733 2796.1293

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**TS<sub>mBPR</sub>**  
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Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000010 0.000008 -0.101850  
6 1.335590 -1.062380 -0.038454  
6 -1.335613 1.062381 -0.038424  
6 -1.062365 -1.335609 -0.038406  
6 1.062396 1.335594 -0.038472  
8 -1.783761 -2.242598 0.071337  
8 2.242556 -1.783808 0.071258  
8 -2.242575 1.783812 0.071304  
8 1.783858 2.242535 0.071226  
1 0.000014 0.000024 1.267362

*Frequencies, cm<sup>-1</sup>*

-182.8092 103.3793 103.3797  
117.5562 118.5660 307.7573  
449.2607 449.2610 495.0303  
527.3609 527.3610 552.9617

587.0342 633.6327 732.8709  
 732.8710 759.3112 974.2097  
 974.2098 1994.8022 1994.8024  
 2041.1749 2058.0741 2577.3389

---

**TS<sub>OSH</sub>**

---

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000112 -0.000018 -0.298914  
 6 0.000435 1.218553 0.826251  
 6 0.000432 -1.218471 0.826377  
 6 1.625665 -0.000041 -0.764173  
 6 -1.626332 -0.000037 -0.762655  
 8 2.751878 -0.000056 -1.057418  
 8 0.000814 2.083714 1.607691  
 8 0.000809 -2.083551 1.607907  
 8 -2.752809 -0.000049 -1.054874  
 1 -0.000768 -0.000092 -1.748576

*Frequencies, cm<sup>-1</sup>*

-905.0678 81.4743 99.7134  
 106.5698 108.7806 137.3108  
 475.7347 505.3135 520.4134  
 597.9026 611.6408 612.2310  
 618.9537 637.4645 718.3225  
 730.5852 781.1195 911.2460  
 1072.5826 1990.8506 2012.5896  
 2100.9556 2117.3003 2407.4735

---

**TS<sub>OSL</sub>**

---

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.115176 -0.000618 -0.232134  
 6 -0.118637 0.003367 1.482946  
 6 0.988488 -1.259979 -0.433024  
 6 0.983403 1.262219 -0.438871  
 6 -1.871714 -0.004702 -0.529286  
 8 1.755750 2.131173 -0.538834  
 8 -0.109667 0.006119 2.651948  
 8 1.764360 -2.126244 -0.528954  
 8 -3.019356 -0.007306 -0.690348  
 1 -0.077571 -0.003710 -1.615998

*Frequencies, cm<sup>-1</sup>*

-123.1192 101.2046 103.1714  
 115.8882 126.3228 330.4814  
 420.5241 461.0838 494.5005  
 537.7607 561.9042 576.2962  
 611.0665 672.9236 674.9627

731.7641 850.6324 860.3467  
 1455.3673 2014.9745 2028.5670  
 2084.4289 2485.9794 3318.4634

---

**TS<sub>BFI</sub>**

---

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.000548 0.012511 -0.092001  
 6 0.000049 1.619021 0.686267  
 6 -0.000292 -1.468384 0.719123  
 6 1.575802 -0.034401 -0.698170  
 6 -1.574956 -0.034392 -0.697223  
 8 2.664160 -0.078595 -1.109018  
 8 -0.000321 2.677429 1.164614  
 8 -0.000895 -2.448043 1.364067  
 8 -2.663577 -0.078593 -1.107382  
 1 -0.000114 -0.505834 -1.350156

*Frequencies, cm<sup>-1</sup>*

-600.1872 49.2760 92.1618  
 111.2524 137.3387 161.0617  
 432.8124 447.5158 497.8826  
 532.3572 533.2676 601.7420  
 645.0872 693.8238 706.8349  
 746.0694 916.7356 1016.0012  
 1145.9248 2004.9793 2059.2284  
 2114.2966 2188.5440 2732.9509

**Table S2.** Geometries and  
 Frequencies of HM(CO)<sub>4</sub> Complexes  
 Calculated at B3LYP/LanL2TZ(f)  
 [Fe]/ 6-31G(d,p)[C,O,H] Level (BS-III)  
 Presented in Table 2.

---

**[HCo(CO)<sub>4</sub>]<sup>+</sup> cation-rad**

---

**Quasi-SP**

---

Charge = 1 Multiplicity = 2

*Cartesian Coordinates*

6 0.007867 -1.484053 0.921891  
 6 0.000965 1.438963 0.968727  
 6 -1.825009 -0.016374 -0.786647  
 6 1.817366 -0.008064 -0.803651  
 8 -2.909743 0.035399 -1.104528  
 8 0.014370 -2.341178 1.659461  
 8 0.001286 2.333985 1.659511  
 8 2.898688 0.049409 -1.132074

1 -0.007275 0.964082 -1.415663  
 27 -0.001358 -0.043253 -0.335008

*Frequencies, cm<sup>-1</sup>*

69.4400 77.5265 92.2824  
 93.1962 100.2916 263.4066  
 278.6631 289.3875 329.2224  
 332.7193 364.6907 375.5773  
 429.4661 446.3922 459.0390  
 497.9547 500.1029 715.1711  
 821.0577 1956.3725 2242.4727  
 2251.7009 2255.6180 2279.6716

**EBT**

Charge = 1 Multiplicity = 2

*Cartesian Coordinates*

6 1.871911 0.010501 0.617210  
 6 -1.871745 -0.010439 0.617640  
 6 0.009942 -1.778454 -0.524264  
 6 -0.010038 1.778447 -0.524442  
 8 0.015916 -2.856570 -0.874537  
 8 2.947306 0.016210 0.964201  
 8 -2.947180 -0.016262 0.964507  
 8 -0.016161 2.856525 -0.874828  
 1 0.000043 -0.000056 -1.513551  
 27 0.000018 0.000019 -0.038447

*Frequencies, cm<sup>-1</sup>*

50.4374 81.5608 85.2741  
 85.3200 106.5459 165.1190  
 237.5437 271.6441 299.1417  
 339.7841 345.2202 370.0780  
 379.0744 393.8018 453.0628  
 481.5475 514.7015 526.2845  
 649.4514 1891.9023 2228.2152  
 2245.7036 2250.3858 2271.5159

**TS<sub>mBPR</sub>**

Charge = 1 Multiplicity = 2

*Cartesian Coordinates*

7 -0.000007 0.000011 -0.032923  
 6 0.276593 1.839890 -0.050394  
 6 -0.276572 -1.839872 -0.050520  
 6 1.839874 -0.276585 -0.050373  
 6 -1.839887 0.276581 -0.050539  
 8 2.957526 -0.444778 0.019583  
 8 0.444770 2.957546 0.019551  
 8 -0.444715 -2.957519 0.019654  
 8 -2.957536 0.444722 0.019622

1 -0.000222 -0.000130 1.472607

*Frequencies, cm<sup>-1</sup>*

-250.1640 100.9219 103.4045  
 103.4046 115.0687 125.6749  
 335.6026 335.6029 339.7511  
 362.7000 384.7938 393.1443  
 393.1446 525.0457 539.4130  
 563.4648 563.4652 680.5803  
 680.5807 1721.9758 2228.9679  
 2228.9680 2238.5200 2274.4795

**TS<sub>OSH</sub>**

Charge = 1 Multiplicity = 2

*Cartesian Coordinates*

6 -0.000042 1.441820 0.952826  
 6 -0.000047 -1.441784 0.952880  
 6 1.807328 -0.000017 -0.772071  
 6 -1.807257 -0.000012 -0.772240  
 8 2.907738 -0.000024 -1.038251  
 8 -0.000071 2.328518 1.654620  
 8 -0.000078 -2.328456 1.654708  
 8 -2.907642 -0.000015 -1.038524  
 1 0.000085 -0.000036 -1.895655  
 27 0.000017 -0.000007 -0.375301

*Frequencies, cm<sup>-1</sup>*

-728.4388 75.7076 79.2146  
 91.4100 95.1661 109.4016  
 250.0072 295.3918 305.6936  
 318.6550 324.2303 369.6312  
 392.9750 440.2895 443.8275  
 485.2562 488.7048 521.0749  
 675.1626 1818.9319 2238.7028  
 2249.9614 2252.3076 2277.4496

**TS<sub>OSL</sub>**

Charge = 1 Multiplicity = 2

*Cartesian Coordinates*

6 -0.062061 -0.000208 1.726684  
 6 1.068868 -1.452181 -0.479957  
 6 1.068827 1.452327 -0.479608  
 6 -2.039187 0.000036 -0.522256  
 8 1.746876 2.328292 -0.712990  
 8 -0.012577 -0.000358 2.856785  
 8 1.746941 -2.328070 -0.713550  
 8 -3.131099 0.000056 -0.811279  
 1 -0.121550 0.000205 -1.646282  
 27 -0.107343 0.000022 -0.176838



*Frequencies, cm<sup>-1</sup>*

-297.5944 74.5934 79.1869  
93.7743 99.1028 140.6010  
286.2935 290.7915 307.0726  
307.3215 327.9250 360.3789  
373.7716 449.1269 459.3603  
476.0763 493.5859 766.1428  
845.9635 1981.5106 2236.3447  
2248.9993 2259.7974 2277.9186

**TS<sub>BFI</sub>**

Charge = 1 Multiplicity = 2

*Cartesian Coordinates*

27 0.003849 -0.000002 -0.064282  
6 1.882611 -0.000678 0.634417  
6 -1.831179 0.000636 0.665199  
6 -0.014560 -1.778893 -0.551534  
6 -0.013293 1.778912 -0.551495  
8 -0.033188 -2.856108 -0.904404  
8 2.948128 -0.001029 1.009287  
8 -2.890722 0.001004 1.059497  
8 -0.031157 2.856147 -0.904342  
1 -0.189896 0.000083 -1.524220

*Frequencies, cm<sup>-1</sup>*

-183.2187 70.5641 83.3238  
86.3920 101.5636 119.8841  
238.7531 262.9278 299.0911  
313.4731 341.7236 379.5518  
391.2690 406.2869 450.3319  
477.9620 512.8742 524.2110  
652.8944 1904.2198 2227.4737  
2243.1630 2253.2207 2271.6265

**HFe(CO)<sub>4</sub> radical**

**Quasi-SP**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.006611 -0.009225 -0.265250  
6 -0.001593 -1.404245 0.907154  
6 -0.005645 1.373555 0.931139  
6 -1.766793 -0.021350 -0.732700  
6 1.751439 -0.016680 -0.740885  
8 -2.860751 0.024568 -1.077504  
8 0.002592 -2.285219 1.644213

8 -0.005100 2.280707 1.634961  
8 2.843372 0.032580 -1.091591  
1 -0.009859 0.999956 -1.417344

*Frequencies, cm<sup>-1</sup>*

68.0480 82.7511 93.4196  
97.1487 103.7794 310.2420  
346.6275 363.1107 402.7738  
428.8517 457.9388 461.1624  
486.9833 520.9959 547.9227  
590.4732 593.8184 699.6557  
784.3553 1880.8653 2107.6187  
2111.6781 2116.3567 2178.6741

**EBT**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000223 -0.000103 -0.014160  
6 -0.016365 1.741536 0.433119  
6 0.015615 -1.741778 0.433001  
6 1.773661 0.016376 -0.507579  
6 -1.773767 -0.016483 -0.508789  
8 2.880806 0.027041 -0.811598  
8 -0.026426 2.827006 0.812231  
8 0.025377 -2.827242 0.812144  
8 -2.880648 -0.027026 -0.813772  
1 -0.000741 -0.000235 1.503103

*Frequencies, cm<sup>-1</sup>*

52.1227 91.7354 93.9796  
96.1363 111.3905 323.6540  
365.7682 388.4928 401.7433  
430.2086 463.7844 475.9051  
483.4111 513.2077 567.2086  
593.1565 618.1041 658.1203  
662.7024 1821.7044 2094.8181  
2105.4430 2109.5771 2175.7813

**TS<sub>mBPR</sub>**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000001 -0.000037 -0.038490  
6 1.093655 -1.459283 -0.042489  
6 -1.093666 1.459203 -0.042502  
6 -1.459251 -1.093703 -0.042590  
6 1.459248 1.093632 -0.042643  
8 -2.376803 -1.781799 0.019897  
8 1.781734 -2.376840 0.020035  
8 -1.781756 2.376757 0.020000

8 2.376801 1.781732 0.019785  
1 0.000014 -0.000018 1.467862

*Frequencies, cm<sup>-1</sup>*

-65.7520 98.4436 98.4507  
100.1842 113.2561 334.5877  
359.6445 359.6448 374.8239  
412.1071 433.0700 458.9749  
458.9869 576.1556 627.1593  
627.1619 630.7520 740.5076  
740.5166 1775.2837 2101.1023  
2101.1212 2110.7653 2182.3973

**TS<sub>OSH</sub>**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 0.000037 -0.000147 -0.338082  
6 0.000084 -1.406995 0.843010  
6 -0.000345 1.407687 0.841836  
6 -1.772566 -0.000562 -0.702696  
6 1.772747 -0.000019 -0.702171  
8 -2.886727 -0.000839 -0.978570  
8 0.000146 -2.324018 1.535016  
8 -0.000558 2.325286 1.533077  
8 2.886990 0.000045 -0.977715  
1 0.000261 -0.000806 -1.892808

*Frequencies, cm<sup>-1</sup>*

-465.5721 74.9535 84.6096  
87.4321 100.2837 110.9902  
311.0869 363.1478 366.6586  
404.7570 437.9198 449.5733  
459.5043 529.4611 532.1587  
559.2450 582.5463 610.3565  
695.8868 1802.8527 2101.5699  
2111.7352 2117.1483 2178.9219

**TS<sub>OSL</sub>**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.073003 -0.168041 -0.508665  
6 0.018646 1.311577 0.546719  
6 0.162926 -1.410444 0.785859  
6 1.593915 -0.076877 -1.207093  
6 -1.656966 0.099107 -1.466963  
8 2.631182 -0.052079 -1.701920  
8 0.103609 2.234607 1.225178  
8 0.280868 -2.242006 1.570694  
8 -2.606066 0.163891 -2.104836

1 -0.115303 -1.420864 -1.377788

*Frequencies, cm<sup>-1</sup>*

-333.3162 74.3356 80.1866  
97.3596 102.9099 140.9630  
336.2700 341.3464 344.6080  
384.2402 454.5580 460.0685  
474.5070 527.7419 562.6411  
562.7410 598.7269 733.2257  
798.6824 1897.2077 2098.5248  
2110.4957 2122.0007 2174.7041

**TS<sub>BFI</sub>**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

26 -0.000014 0.020398 -0.083170  
6 -0.001292 1.771205 0.608136  
6 0.001169 -1.629025 0.687782  
6 1.732348 -0.045897 -0.558971  
6 -1.732259 -0.048411 -0.559038  
8 2.811042 -0.115697 -0.951890  
8 -0.002062 2.834424 1.034904  
8 0.001891 -2.658227 1.200095  
8 -2.810837 -0.119774 -0.951996  
1 0.000290 -0.343381 -1.553925

*Frequencies, cm<sup>-1</sup>*

-405.8646 72.6776 80.9818  
94.6905 97.9205 123.4379  
310.3148 357.4550 380.8366  
390.5930 452.9132 467.8474  
469.1837 508.7596 551.1174  
576.6473 580.8332 654.4841  
663.0514 1860.6352 2095.8994  
2103.1288 2115.5695 2173.3239

**[HMn(CO)<sub>4</sub>]<sup>-</sup> anion- radical**

**Quasi-SP**

Charge = -1 Multiplicity = 2

*Cartesian Coordinates*

6 0.000384 1.491015 0.647568  
6 -0.000298 -1.199333 1.045850  
6 1.762187 -0.083174 -0.754389  
6 -1.762203 -0.082343 -0.754335  
8 2.879511 -0.173628 -1.085218  
8 0.000633 2.488047 1.262604

8 -0.000608 -1.974751 1.923322  
 8 -2.879577 -0.172252 -1.085147  
 1 -0.000269 -1.155945 -1.457420  
 25 0.000007 -0.037615 -0.311009

*Frequencies, cm<sup>-1</sup>*

65.0216 81.1124 82.5433  
 94.9032 99.1078 286.0716  
 368.2457 390.7692 442.2408  
 456.3806 489.9244 506.3028  
 512.2743 571.0951 576.9788  
 617.9842 647.8636 703.3766  
 730.8165 1720.7957 1960.1271  
 1967.9448 1972.5344 2056.7840

**EBT**

Charge = -1 Multiplicity = 2

*Cartesian Coordinates*

6 -0.000026 -1.726595 0.583601  
 6 -0.000033 1.726596 0.583599  
 6 -1.724080 -0.000004 -0.514696  
 6 1.724692 0.000003 -0.514598  
 8 -2.799601 -0.000006 -0.976726  
 8 -0.000958 -2.812174 1.022894  
 8 -0.000968 2.812175 1.022890  
 8 2.800311 0.000004 -0.976369  
 1 0.000129 -0.000001 -1.561624  
 25 0.000251 0.000000 -0.000293

*Frequencies, cm<sup>-1</sup>*

59.0524 80.2593 81.4811  
 88.4520 101.5551 350.1425  
 394.9989 418.5764 440.4216  
 445.8090 499.7483 504.6504  
 510.1898 518.6870 589.9505  
 601.3325 658.8628 666.3022  
 715.8117 1767.5227 1943.7304  
 1963.4116 1969.4162 2053.8990

**TS<sub>mBPR</sub>**

Charge = -1 Multiplicity = 2

*Cartesian Coordinates*

25 -0.000006 -0.000001 -0.019924  
 6 1.003307 1.524085 -0.037094  
 6 -1.003306 -1.524097 -0.037111  
 6 1.524090 -1.003302 -0.037071  
 6 -1.524093 1.003311 -0.037135  
 8 2.500388 -1.645997 -0.004447  
 8 1.646019 2.500374 -0.004484

8 -1.646002 -2.500395 -0.004513  
 8 -2.500381 1.646023 -0.004552  
 1 -0.000035 0.000007 1.532533

*Frequencies, cm<sup>-1</sup>*

-64.2653 84.2308 84.2311  
 95.2880 98.7065 354.3502  
 354.3505 393.7494 422.8184  
 438.1595 460.7438 498.1306  
 498.1307 591.4003 642.6498  
 642.6498 691.2180 756.3984  
 756.3984 1727.1576 1959.7542  
 1959.7547 1975.5014 2063.6753

**TS<sub>OSH</sub>**

Charge = -1 Multiplicity = 2

*Cartesian Coordinates*

6 0.000053 -1.383361 0.806021  
 6 0.000048 1.383363 0.806018  
 6 -1.781716 -0.000004 -0.689740  
 6 1.781626 0.000003 -0.689973  
 8 -2.915948 -0.000006 -0.967873  
 8 0.000105 -2.297531 1.539707  
 8 0.000097 2.297534 1.539703  
 8 2.915822 0.000004 -0.968256  
 1 -0.000126 -0.000003 -1.955817  
 25 -0.000022 0.000000 -0.343375

*Frequencies, cm<sup>-1</sup>*

-280.6900 72.6428 76.3306  
 84.2247 98.7804 103.9180  
 372.2450 380.0726 395.0678  
 448.2366 488.4532 493.1989  
 496.9976 564.9674 577.0403  
 616.1203 618.5475 680.0317  
 698.4240 1675.0156 1951.4125  
 1972.0052 1973.9407 2056.8114

**TS<sub>OSL</sub>**

Charge = -1 Multiplicity = 2

*Cartesian Coordinates*

6 -0.084196 -0.000033 1.612738  
 6 -0.962337 1.378851 -0.523546  
 6 -0.962338 -1.378828 -0.523602  
 6 1.974833 0.000006 -0.356364  
 8 -1.638601 -2.296081 -0.794212  
 8 -0.254949 -0.000058 2.771519  
 8 -1.638599 2.296117 -0.794116  
 8 3.123939 0.000010 -0.562257

1 0.274378 0.000026 -1.767079  
25 0.127821 0.000004 -0.178230

*Frequencies, cm<sup>-1</sup>*

-292.8484 64.9256 79.5026  
91.2298 98.6845 151.1285  
340.8643 345.7747 377.5434  
432.0123 491.4017 513.5292  
523.4545 562.3262 599.5688  
608.9842 641.0250 673.8090  
747.4743 1735.1713 1956.0377  
1962.2346 1974.6826 2051.5162

-----  
**TS<sub>BFI</sub>**  
-----

Charge = -1 Multiplicity = 2

*Cartesian Coordinates*

25 -0.000012 0.046834 -0.094690  
6 -0.000650 1.764493 0.598467  
6 0.000494 -1.539170 0.745789  
6 1.723604 -0.091642 -0.595491  
6 -1.723476 -0.092832 -0.595687  
8 2.801568 -0.219172 -1.033841  
8 -0.001049 2.827103 1.084958  
8 0.000821 -2.533945 1.368446  
8 -2.801303 -0.221105 -1.034157  
1 0.000177 -0.238995 -1.634458

*Frequencies, cm<sup>-1</sup>*

-416.4530 70.3833 71.8266  
91.5125 92.2601 123.2542  
345.9636 390.1869 410.9753  
435.8541 460.2697 501.6662  
508.3719 516.3111 579.5925  
596.6816 616.1231 655.0111  
724.4579 1769.0405 1945.0091  
1965.4975 1968.7652 2050.9134

-----  
**HRu(CO)<sub>4</sub> radical**  
-----

**Quasi-SP**  
-----

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

44 0.000125 -0.033658 -0.303233  
6 -0.002340 1.667705 0.776992  
6 0.001370 -1.319737 1.139214  
6 1.933509 -0.068860 -0.700163  
6 -1.932957 -0.073656 -0.701175

8 3.048955 -0.166574 -0.954671  
8 -0.003776 2.640551 1.384892  
8 0.002236 -2.107126 1.977230  
8 -3.048040 -0.174102 -0.956213  
1 0.001994 -1.293761 -1.356854

*Frequencies, cm<sup>-1</sup>*

66.1846 76.4920 84.0686  
85.4979 88.0250 282.7992  
319.5381 331.0357 379.1307  
396.0841 417.1568 419.2673  
459.6503 463.2900 492.8331  
496.5159 544.5537 725.0717  
806.2231 1935.9864 2097.5360  
2099.9096 2115.0465 2171.5152

-----  
**SP**  
-----

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

44 -0.000037 -0.000007 -0.003494  
6 -0.422976 1.923186 -0.035998  
6 0.423025 -1.923173 -0.036000  
6 1.923177 0.422886 -0.044438  
6 -1.923248 -0.422903 -0.044424  
8 3.045635 0.669366 -0.023127  
8 -0.669650 3.045367 -0.006435  
8 0.669945 -3.045301 -0.006436  
8 -3.045706 -0.669388 -0.023187  
1 -0.000034 -0.000010 1.592353

*Frequencies, cm<sup>-1</sup>*

40.7677 88.5637 88.5964  
91.4161 97.1579 349.5710  
353.1429 353.5042 387.0087  
387.3309 387.4550 436.6643  
442.9473 511.2052 584.4398  
584.5754 612.8624 728.8229  
730.3296 1976.0142 2090.2826  
2090.6919 2100.1618 2181.7865

-----  
**TS<sub>OSH</sub>**  
-----

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

44 0.000083 -0.000135 -0.327973  
6 0.000090 -1.458512 0.989886  
6 -0.000352 1.459328 0.988672  
6 -1.937463 -0.000571 -0.671089  
6 1.937706 0.000015 -0.670617  
8 -3.057231 -0.000842 -0.918939

8 -0.000034 -2.356375 1.708560  
 8 -0.000747 2.357787 1.706601  
 8 3.057535 0.000082 -0.918195  
 1 0.000290 -0.000831 -2.014501

*Frequencies, cm<sup>-1</sup>*

-622.9631 72.1226 77.3597  
 79.5790 87.2012 95.7327  
 294.4713 327.7570 329.1120  
 395.6521 399.0970 407.8811  
 441.7169 467.2839 484.3950  
 490.4278 512.5324 559.8799  
 694.8221 1802.1826 2083.9345  
 2104.7085 2112.0560 2174.4988

**TS<sub>OSL</sub>**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

44 0.121643 0.000011 -0.176617  
 6 -0.037866 -0.000197 1.830541  
 6 -1.133294 1.426055 -0.521524  
 6 -1.133358 -1.425893 -0.521912  
 6 2.154108 -0.000006 -0.348144  
 8 -1.858344 -2.283538 -0.773987  
 8 -0.155755 -0.000313 2.971290  
 8 -1.858271 2.283778 -0.773356  
 8 3.282283 0.000010 -0.555562  
 1 0.270852 0.000266 -1.809688

*Frequencies, cm<sup>-1</sup>*

-226.9827 69.5945 73.8795  
 86.7519 91.1742 151.6720  
 303.5481 304.1616 329.0778  
 364.3132 383.2937 435.9622  
 441.1800 472.8172 488.4920  
 514.4846 526.2805 743.5420  
 818.5857 1946.2193 2082.7445  
 2102.8899 2109.4732 2165.4515

**TS<sub>BFI</sub>**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

44 0.000004 -0.005444 -0.139713  
 6 -0.001024 1.922165 0.582758  
 6 0.000933 -1.770512 0.615467  
 6 1.943424 -0.024946 -0.423215  
 6 -1.943390 -0.027008 -0.423247  
 8 3.066009 -0.073947 -0.656820  
 8 -0.001605 3.014711 0.937852

8 0.001489 -2.825138 1.081777  
 8 -3.065918 -0.077199 -0.656871  
 1 0.000367 -0.666071 -1.610726

*Frequencies, cm<sup>-1</sup>*

-331.7625 71.4728 74.5165  
 86.0344 91.0813 114.1980  
 297.2255 316.3553 353.5473  
 356.4380 394.7055 441.4193  
 444.4357 474.9329 522.9866  
 532.5277 552.4514 687.3630  
 759.2138 1962.9193 2081.5569  
 2090.9653 2103.8138 2173.3983

**HOs(CO)<sub>4</sub> radical**

**Quasi-SP**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

6 -0.007631 -1.509883 1.037974  
 6 -0.001095 1.440380 1.023684  
 6 -1.923904 -0.024409 -0.612800  
 6 1.928825 -0.032838 -0.596846  
 8 -3.041824 -0.005274 -0.885902  
 8 -0.012708 -2.407863 1.757858  
 8 -0.002484 2.301482 1.791715  
 8 3.049062 -0.018691 -0.860601  
 1 0.008645 1.097034 -1.510854  
 76 0.001024 0.009293 -0.237181

*Frequencies, cm<sup>-1</sup>*

73.7911 85.5891 86.2103  
 91.5780 93.9410 335.2394  
 364.8970 386.6812 431.1966  
 431.4057 478.0731 490.0431  
 496.0861 500.3302 528.9445  
 531.8428 581.9564 712.1289  
 833.5888 2019.4839 2088.7333  
 2091.2180 2114.6227 2173.2487

**SP**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

76 -0.000011 0.000007 0.019111  
 6 1.751058 0.885772 -0.038642  
 6 -1.751043 -0.885809 -0.038879  
 6 0.885722 -1.750849 -0.044595

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.885704 | 1.750881  | -0.044578 |
| 8 | 1.405833  | -2.778565 | -0.070774 |
| 8 | 2.778919  | 1.405744  | -0.059499 |
| 8 | -2.778875 | -1.405845 | -0.059583 |
| 8 | -1.405775 | 2.778617  | -0.070756 |
| 1 | -0.000187 | -0.000088 | 1.632609  |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| 40.1579   | 89.9208   | 89.9305   |
| 92.9318   | 97.9492   | 383.3336  |
| 385.2793  | 385.3652  | 415.9746  |
| 416.0626  | 477.5433  | 485.0848  |
| 494.3839  | 532.5846  | 607.0907  |
| 607.1616  | 628.9579  | 749.3773  |
| 750.8912  | 2080.0897 | 2080.3647 |
| 2096.7175 | 2153.8683 | 2190.9361 |

**TS<sub>OSH</sub>**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | 0.000073  | -1.433647 | 1.038172  |
| 6  | -0.000361 | 1.434489  | 1.036984  |
| 6  | -1.938737 | -0.000506 | -0.555817 |
| 6  | 1.938914  | 0.000079  | -0.555288 |
| 8  | -3.065498 | -0.000745 | -0.784856 |
| 8  | 0.000026  | -2.325610 | 1.770853  |
| 8  | -0.000679 | 2.327067  | 1.768914  |
| 8  | 3.065740  | 0.000180  | -0.784014 |
| 1  | 0.000274  | -0.000830 | -1.956161 |
| 76 | 0.000049  | -0.000116 | -0.257833 |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| -555.4435 | 81.2454   | 82.3276   |
| 89.2603   | 97.2650   | 99.9804   |
| 365.3315  | 372.9889  | 383.8884  |
| 433.9668  | 470.6701  | 481.3299  |
| 491.6917  | 512.1984  | 528.3136  |
| 532.2548  | 541.2292  | 592.8106  |
| 762.5412  | 1955.5784 | 2071.9091 |
| 2093.7348 | 2100.0546 | 2172.3065 |

**TS<sub>OSL</sub>**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

|    |           |           |           |
|----|-----------|-----------|-----------|
| 76 | 0.093936  | 0.000202  | -0.153623 |
| 6  | -0.053943 | -0.000421 | 1.824800  |
| 6  | -1.170325 | 1.409010  | -0.458435 |
| 6  | -1.169888 | -1.408903 | -0.458473 |
| 6  | 2.087821  | 0.000088  | -0.272604 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | -1.885304 | -2.289069 | -0.671146 |
| 8 | -0.154373 | -0.000783 | 2.970642  |
| 8 | -1.885898 | 2.288997  | -0.671280 |
| 8 | 3.230895  | -0.000972 | -0.417845 |
| 1 | 0.256326  | 0.000625  | -1.819326 |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| -210.3816 | 77.5211   | 82.9249   |
| 91.2628   | 98.2593   | 187.7827  |
| 345.5270  | 348.0925  | 384.5258  |
| 428.1662  | 432.9133  | 492.8865  |
| 493.8339  | 514.4905  | 528.2246  |
| 548.0803  | 561.0562  | 738.8950  |
| 817.9348  | 2020.2504 | 2077.3066 |
| 2079.0974 | 2108.0605 | 2166.3343 |

**TS<sub>BFI</sub>**

Charge = 0 Multiplicity = 2

*Cartesian Coordinates*

|    |           |           |           |
|----|-----------|-----------|-----------|
| 76 | -0.000003 | -0.000957 | -0.123590 |
| 6  | -0.000962 | 1.870245  | 0.614688  |
| 6  | 0.000898  | -1.743164 | 0.650761  |
| 6  | 1.942423  | -0.026575 | -0.381659 |
| 6  | -1.942390 | -0.028709 | -0.381657 |
| 8  | 3.069410  | -0.069669 | -0.605516 |
| 8  | -0.001450 | 2.949169  | 1.022909  |
| 8  | 0.001369  | -2.768225 | 1.188372  |
| 8  | -3.069328 | -0.073044 | -0.605518 |
| 1  | 0.000367  | -0.663907 | -1.621939 |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| -355.3572 | 73.6396   | 82.8138   |
| 88.0009   | 98.6210   | 126.6041  |
| 350.9628  | 361.9240  | 393.3972  |
| 417.9485  | 426.9552  | 491.4134  |
| 502.4760  | 508.2615  | 552.3531  |
| 556.8408  | 582.0275  | 705.1918  |
| 795.1908  | 2059.5373 | 2075.9145 |
| 2096.5527 | 2109.2165 | 2175.3688 |

**HMn(CO)<sub>4</sub> molecule**

**Quasi-SP**

Charge = 0 Multiplicity = 1

*Cartesian Coordinates*

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.005588 | -1.454958 | 0.853035  |
| 6 | 0.000034  | 1.217437  | 0.789356  |
| 6 | -1.818435 | 0.075133  | -0.703475 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | 1.823241  | 0.070212  | -0.691179 |
| 8  | -2.928212 | 0.255493  | -0.941022 |
| 8  | -0.010504 | -2.291941 | 1.644165  |
| 8  | -0.000403 | 2.096495  | 1.534744  |
| 8  | 2.935264  | 0.252419  | -0.916457 |
| 1  | 0.006571  | 0.903701  | -1.629217 |
| 25 | 0.001150  | -0.114015 | -0.417146 |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| 72.5988   | 85.3505   | 93.7433   |
| 104.1777  | 107.0174  | 330.7283  |
| 363.9309  | 366.9225  | 415.8678  |
| 454.7496  | 462.6067  | 488.4348  |
| 541.7969  | 566.4113  | 579.1612  |
| 632.5847  | 635.9638  | 713.8100  |
| 768.2504  | 1807.7766 | 2082.3300 |
| 2094.0241 | 2095.3478 | 2169.0381 |

**SP**

Charge = 0 Multiplicity = 1

*Cartesian Coordinates*

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | -0.012601 | -1.844222 | 0.008329  |
| 6  | 0.007246  | 1.838335  | -0.072316 |
| 6  | -1.842645 | 0.014299  | 0.109982  |
| 6  | 1.832977  | -0.013950 | -0.211617 |
| 8  | -2.953609 | 0.033851  | 0.408581  |
| 8  | 0.002071  | -2.969608 | 0.248420  |
| 8  | 0.031772  | 2.973557  | 0.113532  |
| 8  | 2.979133  | -0.012303 | -0.110981 |
| 1  | 0.112766  | 0.022441  | 1.292813  |
| 25 | -0.019902 | -0.007728 | -0.223020 |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| 23.1577   | 92.5243   | 92.9595   |
| 99.1361   | 114.2543  | 346.0267  |
| 348.2943  | 374.8868  | 416.7433  |
| 418.1208  | 464.9400  | 466.9728  |
| 508.0066  | 584.1391  | 639.0742  |
| 639.4930  | 671.7391  | 803.9425  |
| 805.2343  | 1903.8306 | 2078.6563 |
| 2079.0742 | 2101.0357 | 2173.1780 |

**TS<sub>OSH</sub>**

Charge = 0 Multiplicity = 1

*Cartesian Coordinates*

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 0.000102  | -1.284890 | 0.844720  |
| 6 | -0.000285 | 1.285583  | 0.843667  |
| 6 | -1.834912 | -0.000561 | -0.697999 |
| 6 | 1.835128  | -0.000012 | -0.697543 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -2.966281 | -0.000812 | -0.890938 |
| 8  | 0.000037  | -2.166463 | 1.587791  |
| 8  | -0.000617 | 2.167769  | 1.586010  |
| 8  | 2.966554  | 0.000075  | -0.890165 |
| 1  | 0.000378  | -0.000850 | -2.053090 |
| 25 | 0.000075  | -0.000177 | -0.433823 |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| -380.9771 | 82.9870   | 87.2574   |
| 103.3166  | 105.7387  | 116.4136  |
| 364.5258  | 366.3560  | 366.9892  |
| 415.8678  | 439.8789  | 466.0843  |
| 502.5818  | 548.2949  | 580.6294  |
| 594.6106  | 635.5723  | 686.2438  |
| 720.2734  | 1727.4729 | 2078.1689 |
| 2090.9796 | 2104.9654 | 2171.8340 |

**TS<sub>OSL</sub>**

Charge = 0 Multiplicity = 1

*Cartesian Coordinates*

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | -0.134694 | -0.004448 | 1.724589  |
| 6  | -0.994047 | 1.283998  | -0.505613 |
| 6  | -0.994853 | -1.280667 | -0.512286 |
| 6  | 2.115255  | 0.000582  | -0.480534 |
| 8  | -1.701757 | -2.143672 | -0.808104 |
| 8  | -0.409263 | -0.007421 | 2.843474  |
| 8  | -1.700374 | 2.149023  | -0.796872 |
| 8  | 3.175331  | 0.001336  | -0.910168 |
| 1  | 0.358281  | 0.004059  | -1.660046 |
| 25 | 0.191210  | 0.000201  | -0.092941 |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| -336.0439 | 71.2172   | 80.6102   |
| 101.8544  | 108.1171  | 128.8965  |
| 335.0062  | 340.8327  | 360.4301  |
| 370.4718  | 442.4400  | 485.4284  |
| 511.8904  | 530.2632  | 553.1416  |
| 621.0926  | 660.0526  | 703.2108  |
| 780.9770  | 1805.0246 | 2070.5625 |
| 2075.7836 | 2111.6160 | 2165.1328 |

**TS<sub>BFI</sub>**

Charge = 0 Multiplicity = 1

*Cartesian Coordinates*

|    |           |           |           |
|----|-----------|-----------|-----------|
| 25 | -0.000059 | 0.063241  | -0.113657 |
| 6  | -0.000918 | 1.921987  | 0.611785  |
| 6  | 0.000802  | -1.575753 | 0.616912  |
| 6  | 1.772603  | -0.110735 | -0.536742 |
| 6  | -1.772579 | -0.112473 | -0.536181 |
| 8  | 2.844003  | -0.279314 | -0.927767 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | -0.001164 | 2.939425  | 1.128818  |
| 8 | 0.001325  | -2.600046 | 1.152986  |
| 8 | -2.843937 | -0.282084 | -0.926873 |
| 1 | 0.000203  | -0.543029 | -1.510547 |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| -477.0812 | 57.7446   | 71.4861   |
| 100.3468  | 101.5870  | 111.5049  |
| 315.1969  | 344.6206  | 357.1282  |
| 384.2843  | 454.6197  | 455.9880  |
| 496.5210  | 545.2396  | 578.0036  |
| 600.5152  | 626.7145  | 748.0606  |
| 783.2301  | 1934.7896 | 2059.4974 |
| 2073.7820 | 2118.6125 | 2178.4315 |

**HCo(CO)<sub>4</sub> molecule**

**Quasi-TBP**

Charge = 0 Multiplicity = 1

*Cartesian Coordinates*

|    |           |           |           |
|----|-----------|-----------|-----------|
| 1  | 0.003304  | 0.000680  | -1.668185 |
| 27 | 0.000311  | -0.000212 | -0.189526 |
| 6  | -0.004400 | -0.001692 | 1.617035  |
| 6  | 1.419121  | -1.071382 | -0.459149 |
| 6  | -1.636412 | -0.691150 | -0.466068 |
| 6  | 0.221166  | 1.763710  | -0.459780 |
| 8  | -0.007601 | -0.002729 | 2.762434  |
| 8  | 0.361127  | 2.878838  | -0.692820 |
| 8  | 2.316674  | -1.747777 | -0.692191 |
| 8  | -2.671267 | -1.127317 | -0.703276 |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| 66.9070   | 67.2561   | 96.0268   |
| 96.2251   | 106.7835  | 338.5069  |
| 338.5622  | 349.8822  | 417.1907  |
| 423.4022  | 423.9839  | 466.2012  |
| 506.1333  | 506.5025  | 559.4851  |
| 571.2784  | 571.4117  | 773.2286  |
| 773.7366  | 1997.0483 | 2121.1796 |
| 2121.3877 | 2142.4476 | 2192.2420 |

**TS<sub>BPR</sub>**

Charge = 0 Multiplicity = 1

*Cartesian Coordinates*

|    |           |           |           |
|----|-----------|-----------|-----------|
| 1  | -0.052579 | -0.023835 | 1.672708  |
| 27 | -0.004769 | -0.002225 | 0.153290  |
| 6  | -1.780776 | 0.010118  | -0.120869 |
| 6  | 0.010338  | 1.784384  | -0.039797 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.006286 | -1.782719 | -0.090316 |
| 6 | 1.784934  | -0.008196 | -0.008961 |
| 8 | -2.923852 | 0.017121  | -0.224602 |
| 8 | 2.932278  | -0.012889 | -0.040747 |
| 8 | 0.017621  | 2.930987  | -0.091622 |
| 8 | -0.009537 | -2.927420 | -0.174512 |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| -192.1987 | 101.6475  | 102.2351  |
| 102.2511  | 116.3070  | 178.7146  |
| 357.8278  | 357.8331  | 370.4313  |
| 421.8593  | 440.7414  | 462.2406  |
| 462.2576  | 552.5110  | 616.0508  |
| 616.0684  | 628.0113  | 655.4265  |
| 655.4375  | 1763.7055 | 2117.2016 |
| 2117.2233 | 2122.7036 | 2188.8293 |

**TS<sub>OSH</sub>**

Charge = 0 Multiplicity = 1

*Cartesian Coordinates*

|    |           |           |           |
|----|-----------|-----------|-----------|
| 1  | 0.000120  | -0.000755 | -1.686898 |
| 27 | 0.000027  | -0.000085 | -0.189329 |
| 6  | -1.694457 | -0.000545 | -0.711506 |
| 6  | -0.000350 | 1.513947  | 0.815133  |
| 6  | 0.000049  | -1.513211 | 0.816503  |
| 6  | 1.694801  | -0.000099 | -0.710870 |
| 8  | -2.776183 | -0.000861 | -1.097411 |
| 8  | 2.776665  | -0.000131 | -1.096368 |
| 8  | -0.000637 | 2.474604  | 1.442220  |
| 8  | 0.000015  | -2.473299 | 1.444461  |

*Frequencies, cm<sup>-1</sup>*

|           |           |           |
|-----------|-----------|-----------|
| -322.7462 | 67.4825   | 85.3093   |
| 97.7075   | 108.1201  | 110.9899  |
| 329.4634  | 349.0703  | 371.6325  |
| 412.9894  | 415.8638  | 470.1476  |
| 486.9389  | 496.1336  | 526.0941  |
| 549.0666  | 583.1324  | 618.9726  |
| 636.0568  | 1885.6404 | 2121.9183 |
| 2122.6343 | 2129.8936 | 2186.9533 |



