

SUPPORTING INFORMATION

“Mechanism of Iron Carbonyl-Catalyzed Hydrogenation of Ethylene. I. Theoretical Exploration of Molecular Pathways”

Rubik Asatryan, and Eli Ruckenstein

Department of Chemical and Biological
Engineering, State University of New York
Buffalo, NY, 14260

Calculation Results at B3LYP/
LanL2DZ [Fe]/ 6-311+G(2d,p) [C,H,O]
Level

Table S1. Geometries and
Frequencies of Simple Iron-
Carbonyl Hydrogenates
from Table5

Cis-H₂Fe(CO)₃

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.000153	-0.259485	-0.206163
1	0.000186	-0.294548	1.244621
6	1.747100	-0.608004	0.006529
6	-1.746406	-0.609910	0.006551
6	-0.000858	1.551339	-0.060726
8	2.820286	-0.910397	0.236088
8	-2.819259	-0.913481	0.236118
8	-0.001548	2.677570	0.105709
1	0.000979	-1.788917	-0.221836

Frequencies, cm⁻¹

89.4613	91.4504	101.0994
269.7691	354.5569	374.6847
438.6604	482.3899	491.1252
569.1959	589.0855	595.8830
703.5722	747.0984	769.9794
832.3920	1876.2222	2075.5693
2089.5761	2096.8303	2163.4536

Trans-H₂Fe(CO)₃

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.000061	-0.421454	0.152135
6	-1.805967	-0.518876	-0.002476
6	1.806096	-0.518708	-0.002485
6	-0.000020	1.304369	-0.071931
8	-2.931623	-0.576016	-0.139263
8	2.931757	-0.575743	-0.139278
8	-0.000074	2.439819	-0.182537
1	0.000042	0.058894	1.589080
1	0.000090	-1.136004	-1.227400

Frequencies, cm⁻¹

54.0155	95.3301	102.5896
180.1378	324.4044	371.3269
423.1128	435.8955	460.4477
503.2894	580.3025	605.2415
607.1053	677.1091	733.5687
744.3483	1639.2757	1887.8396
2089.0162	2109.3876	2167.2679

Gauche-H₂Fe(CO)₃

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.000465	-0.042789	0.631742
1	0.958850	0.745950	1.481922
6	1.465155	-0.811845	-0.164729
6	-0.000707	1.465234	-0.222885
6	-1.463935	-0.813321	-0.163827
8	2.417793	-1.208651	-0.640963
8	-0.001666	2.496698	-0.710190
8	-2.416480	-1.211048	-0.639481
1	-0.958151	0.745007	1.482528

Frequencies, cm⁻¹

76.6160	89.4139	99.7946
296.9920	331.2669	337.7925
423.8576	461.4548	525.7211
528.3350	537.9266	588.3728
699.7370	738.9906	763.1589
861.5282	1884.6606	1934.6736
2090.4159	2105.5626	2157.1513

³Fe(CO)₃(H₂)-angular -Triplet

Charge = 0 Multiplicity = 3

Cartesian Coordinates

26 0.003597 -0.018185 0.660490
6 1.588240 -0.544827 -0.141188
6 -0.284922 1.578297 -0.216004
6 -1.240356 -1.058881 -0.229924
8 2.548816 -0.855057 -0.673129
8 -0.452409 2.541252 -0.808243
8 -2.002120 -1.690346 -0.800212
1 -0.577340 -0.048610 2.399054
1 -0.648224 0.707091 2.203562

Frequencies, cm⁻¹

67.3035 70.1217 85.1308
156.3474 215.5709 268.6604
307.2415 331.2175 390.7991
399.8417 437.7457 443.5906
504.5718 518.6538 520.7774
663.7064 1109.8792 2043.1593
2047.0193 2125.3330 3760.2967

³Fe(CO)₃(H₂)-planar -Triplet

Charge = 0 Multiplicity = 3

Cartesian Coordinates

26 -0.000312 -0.270135 0.187828
1 0.394522 -0.250715 1.949872
6 1.786682 -0.705025 -0.127837
6 0.001563 1.558228 -0.038274
6 -1.788071 -0.701605 -0.128234
8 2.877744 -0.937086 -0.362172
8 0.002789 2.695530 -0.152187
8 -2.879524 -0.931601 -0.362782
1 -0.395526 -0.250092 1.949780

Frequencies, cm⁻¹

59.8588 73.4049 82.0246
231.9829 245.9568 308.3448
327.9493 372.6137 409.1109
435.4327 448.3113 456.0923
474.7478 504.4918 518.9185
679.6607 1164.4105 2048.4381
2054.1569 2133.1842 3669.5899

Fe(CO)₃(H₂)-angular

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26 -0.000187 -0.296356 -0.522914
1 -0.411226 -1.702949 -1.350785
6 -1.596361 -0.532386 0.217922
6 0.000859 1.434415 -0.097713
6 1.595719 -0.533962 0.217951
8 -2.539788 -0.721850 0.841309
8 0.001470 2.558939 0.100887
8 2.538976 -0.724206 0.841362
1 0.409518 -1.703255 -1.350883

Frequencies, cm⁻¹

69.4715 94.1996 102.2963
267.8728 319.9040 356.4705
443.1637 443.7611 459.7160
493.0042 541.7291 591.7780
614.0229 632.6401 659.5644
986.1125 1628.8966 2029.9092
2052.0382 2119.3394 3247.2244

Fe(CO)₃(H₂)-planar

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26 0.001112 -0.412160 -0.002876
6 -1.820795 -0.547902 -0.065897
6 -0.001977 1.362141 -0.010917
6 1.823480 -0.542585 -0.066313
8 -2.952890 -0.645926 -0.136702
8 -0.006430 2.499745 0.130914
8 2.955896 -0.636765 -0.137069
1 0.002172 -0.950410 1.422080
1 0.002962 -1.720772 0.913033

Frequencies, cm⁻¹

57.1093 71.5888 93.3821
240.9239 316.4196 354.5748
403.4182 443.5436 450.0974
478.8451 561.1707 606.0346
614.0869 718.4904 792.3509
876.7150 1830.2514 2048.1407
2073.7068 2140.5377 2308.6789

Trans-H₂Fe(CO)₃-Triplet

Charge = 0 Multiplicity = 3

Cartesian Coordinates

26	-0.001933	-0.253646	0.000000
6	-0.002734	-0.527229	1.786287
6	-0.002734	-0.527229	-1.786287
6	0.005045	1.630758	0.000000
8	-0.003316	-0.781072	2.930039
8	-0.003316	-0.781072	-2.930039
8	0.011242	2.802150	0.000000
1	-1.037177	-1.414634	0.000000
1	1.028620	-1.418908	0.000000

Frequencies, cm^{-1}

85.1900	92.6080	109.3892
218.1118	293.0114	354.2264
367.0924	393.5571	413.1457
439.0086	475.4484	551.6173
582.9777	587.3097	620.3319
643.3716	1707.3107	1709.6135
1975.9057	1985.0418	2049.6484

Table S2. Geometries and Frequencies of Reagents and Products

$\text{Fe}(\text{CO})_3(\eta^2\text{-C}_2\text{H}_4)$

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.000125	0.114545	-0.289459
6	-1.509093	-0.868026	-0.495600
6	-0.000735	-0.111454	1.447073
6	1.508906	-0.868955	-0.494598
8	-2.460681	-1.487407	-0.623092
8	-0.001147	-0.202319	2.586604
8	2.460198	-1.488986	-0.621102
6	0.704497	2.042801	-0.365824
1	1.248283	2.174583	-1.297691
1	1.262986	2.336609	0.514211
6	-0.702631	2.043440	-0.365597
1	-1.260510	2.337735	0.514666
1	-1.246639	2.175772	-1.297248

Frequencies, cm^{-1}

68.8572	72.8023	93.9813
105.0805	107.0966	109.4274
359.3719	370.9716	423.5365
426.5527	440.6938	450.8502
463.6239	503.6984	541.3374
575.3075	597.1716	677.1158
803.8134	885.8805	929.7865
944.6103	1219.1460	1231.5801

1465.4215	1531.9165	2054.5454
2056.5268	2117.1431	3097.8235
3109.7107	3176.2320	3199.3010

$^3\text{Fe}(\text{CO})_3(\eta^2\text{-C}_2\text{H}_4)$ –Triplet

Charge = 0 Multiplicity = 3

Cartesian Coordinates

26	0.126341	-0.012495	-0.194076
6	-0.985679	1.450609	-0.496523
6	0.123152	0.058667	1.647518
6	-1.045312	-1.447222	-0.386578
8	-1.664936	2.353481	-0.663582
8	0.080891	0.104260	2.789919
8	-1.763930	-2.329345	-0.485914
6	1.928963	-0.089578	-1.426284
1	1.834551	-1.033957	-1.950291
1	1.859478	0.809470	-2.028089
6	2.392977	-0.041973	-0.144610
1	2.683508	0.894064	0.315775
1	2.659401	-0.943525	0.392732

Frequencies, cm^{-1}

38.2541	48.9689	65.3077
75.9282	79.7515	99.5573
248.9586	293.3105	313.8029
322.3897	367.4111	382.8360
417.8510	443.0940	481.8230
499.8166	518.6272	523.4307
824.3927	914.4394	956.9983
996.2300	1237.9212	1305.9282
1470.0376	1589.0649	2035.2574
2038.6740	2108.4139	3124.1939
3142.8299	3202.7108	3231.9692

$\text{Fe}(\text{CO})_3$

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.495041	-0.388261	0.000000
6	-0.511667	0.293617	1.657614
6	-0.511667	0.293617	-1.657614
6	1.250019	-0.519187	0.000000
8	-0.489551	0.891531	2.635352
8	-0.489551	0.891531	-2.635352
8	2.387074	-0.651125	0.000000

Frequencies, cm^{-1}

64.8314	94.9006	96.9532
325.1534	344.0066	370.6261

434.8736 464.5703 476.3441
526.5635 601.6584 623.6468
2022.6782 2035.8837 2113.6774

³Fe(CO)₃-Triplet

Charge = 0 Multiplicity = 3

Cartesian Coordinates

26 -0.048064 -0.079611 -0.258278
6 1.442856 -0.834484 0.527945
6 -1.460388 -0.807891 0.682893
6 -0.002300 1.680503 0.299878
8 2.348733 -1.286742 1.057664
8 -2.313050 -1.244135 1.306120
8 0.028644 2.753904 0.690470

Frequencies, cm⁻¹

66.3342 67.2896 77.9238
296.4323 300.7710 311.1813
397.0971 437.5241 437.6504
497.7898 498.8040 500.9003
2032.9492 2033.5821 2128.7907

C₂H₄

Charge = 0 Multiplicity = 1

Cartesian Coordinates

6 -0.331259 -0.574064 0.000000
1 0.183544 -1.528142 0.000000
1 -1.414901 -0.605773 0.000000
6 0.331259 0.574064 0.000000
1 -0.183544 1.528142 0.000000
1 1.414901 0.605773 0.000000

Frequencies, cm⁻¹

838.4873 972.5189 975.5829
1057.3351 1247.7162 1379.4895
1477.8888 1686.0357 3124.6712
3137.1848 3195.0498 3223.0856

C₂H₆

Charge = 0 Multiplicity = 1

Cartesian Coordinates

6 -0.381047 -0.663068 0.000000
1 0.303387 -1.514568 0.000010

1 -1.020179 -0.753870 0.881346
6 0.381047 0.663068 0.000000
1 -0.303387 1.514568 0.000010
1 1.020179 0.753870 0.881346
1 1.020164 0.753879 -0.881356
1 -1.020164 -0.753879 -0.881356

Frequencies, cm⁻¹

303.4489 825.1876 826.4400
991.2549 1220.0862 1220.9221
1410.1036 1421.0533 1502.5793
1502.9996 1505.0491 1505.4205
3026.1821 3027.2388 3070.1506
3070.3598 3095.4414 3095.5808

Table S3. Geometries and
Frequencies of Species from Table1

***Trans*-H₂Fe(CO)₃(η²-C₂H₄)**

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26 -0.000025 -0.012211 0.028030
6 -1.740715 0.042636 -0.382490
6 1.740513 0.040943 -0.383172
6 0.001026 1.711278 0.351621
8 -2.824718 0.109519 -0.732825
8 2.824401 0.106930 -0.734075
8 0.001557 2.816804 0.638381
1 -0.001097 0.200270 1.547115
1 0.000146 -0.242753 -1.492968
6 0.680310 -2.135378 0.515567
1 1.232508 -2.017421 1.436966
1 1.228602 -2.504624 -0.340940
6 -0.681948 -2.136086 0.510417
1 -1.223531 -2.505564 -0.350235
1 -1.240991 -2.018796 1.427784

Frequencies, cm⁻¹

50.7585 51.9038 107.3846
117.4990 138.7447 150.2225
249.2304 371.1745 387.2749
458.9229 464.7622 487.0414
522.7166 532.2784 568.4498
604.7710 613.9791 623.1965
640.8356 670.4865 732.5053
790.8983 857.4220 1006.8961
1010.4273 1034.8556 1253.1309
1317.4093 1478.2445 1596.7646
1661.7974 1872.4647 2075.8704
2082.0507 2135.3588 3150.4118

3155.1668 3231.2548 3255.8084

HFe(CO)₃(C₂H₅)-eqax

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26 -0.000064 0.020205 -0.049171
6 -1.747210 -0.068769 -0.455391
6 1.747718 -0.054134 -0.455577
6 -0.007402 1.761832 0.403047
8 -2.820954 -0.141575 -0.831184
8 2.821993 -0.118102 -0.831463
8 -0.012120 2.866960 0.685927
1 0.902807 -1.978215 1.992579
6 0.007100 -1.667183 1.457148
1 0.002006 -0.517349 1.657902
1 -0.885712 -1.986075 1.992797
6 0.008394 -2.003064 -0.002141
1 0.902188 -2.497643 -0.365565
1 -0.881269 -2.505126 -0.365442
1 -0.001303 0.288723 -1.502589

Frequencies, cm⁻¹

72.4282 93.2181 99.9807
124.3111 129.1709 169.8194
350.9727 351.3529 437.7474
439.1256 452.6758 454.7925
477.2891 521.1576 522.2448
564.0431 606.0337 631.9341
727.4376 781.8663 819.8159
872.8835 982.5646 1035.3934
1114.5534 1175.4427 1374.5275
1463.0719 1514.0553 1627.4768
1983.7491 2078.3233 2080.3965
2141.8581 2338.2634 3070.1128
3112.9587 3130.2037 3174.5107

TSrotA

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26 -0.196798 -0.010315 -0.076318
6 -1.134021 1.509053 0.155220
6 0.941731 -1.339705 0.337962
6 -1.634769 -1.089264 -0.315083
8 -1.688029 2.465361 0.427806
8 1.625052 -2.158982 0.736171
8 -2.538706 -1.768835 -0.455246
1 3.228425 0.017982 0.095602

6 2.770344 0.725092 -0.599058
1 2.664740 0.216716 -1.562318
1 3.491163 1.537210 -0.751043
6 1.438427 1.276192 -0.080073
1 1.563498 1.708884 0.914490
1 1.124045 2.099766 -0.732709
1 -0.431929 -0.100915 1.356584

Frequencies, cm⁻¹

-84.2089 58.9693 92.4248
99.9586 111.0870 127.3085
217.5129 280.4652 360.3468
405.5021 422.8772 437.7821
442.8977 481.0100 525.6942
573.6148 596.4750 603.3548
623.8463 743.1918 815.8149
942.2370 984.9266 1012.6684
1198.1248 1280.3227 1413.1043
1457.4079 1497.9334 1505.8719
2057.8916 2082.4923 2087.2573
2151.7125 2987.7261 3000.7627
3041.2705 3062.7226 3084.7663

HFe(CO)₃(C₂H₅)

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26 -0.189027 0.003027 -0.076170
6 -0.993451 1.574443 0.267893
6 0.820658 -1.431173 0.317454
6 -1.713066 -0.933650 -0.379754
8 -1.463736 2.553726 0.609413
8 1.430929 -2.310710 0.706821
8 -2.669711 -1.518200 -0.584709
1 3.167967 0.813798 0.817087
6 2.892443 0.664254 -0.230518
1 3.097847 -0.378395 -0.477522
1 3.571411 1.283918 -0.827262
6 1.441902 1.058699 -0.455773
1 1.342768 2.138947 -0.353925
1 1.106116 0.804250 -1.504896
1 -0.442168 -0.135207 1.358926

Frequencies, cm⁻¹

40.2512 91.5166 92.5663
103.7099 107.0855 156.9563
218.5033 278.0771 334.9094
382.2616 425.2914 443.8091
446.7408 476.1093 525.0736
576.8320 591.1841 609.7803
657.4107 722.5183 806.2533

891.7723	1009.5210	1035.5278
1186.1958	1257.8936	1412.0803
1424.6017	1491.1436	1502.3572
2029.3904	2081.1589	2085.3804
2148.0005	2686.3598	3006.7147
3056.2696	3073.8640	3098.0608

TS2A

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.133975	-0.038319	-0.187847
6	1.198354	-1.462112	0.136063
6	-0.827755	1.454841	0.134253
6	1.600449	0.991177	-0.208529
8	1.864543	-2.334484	0.446151
8	-1.387035	2.398818	0.448089
8	2.537194	1.647872	-0.166065
1	-3.148802	-0.971985	1.101140
6	-2.921056	-0.847650	0.039807
1	-3.148910	0.183537	-0.232711
1	-3.609483	-1.495352	-0.512873
6	-1.481752	-1.226405	-0.257068
1	-1.306582	-2.277913	-0.037713
1	-1.218263	-1.053024	-1.334941
1	-0.578366	-0.545726	1.008562

Frequencies, cm⁻¹

-901.5841	38.3620	96.2674
99.4509	105.0088	111.4231
151.3167	235.2432	278.5944
378.3475	382.7719	434.9735
440.3148	450.9357	492.1111
510.7849	614.3519	630.1344
654.3921	703.5376	831.0184
915.2274	1004.5438	1052.2317
1190.6356	1258.7891	1416.8721
1427.8265	1493.1257	1497.3396
2023.0211	2057.7846	2061.8545
2131.5631	2739.5431	3018.8890
3069.1636	3090.6965	3110.7571

HFe(CO)₃(C₂H₅)(η^2 -C₂H₄)

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.187042	-0.000394	-0.094452
6	0.180060	-1.724101	-0.366213
6	0.173444	1.725570	-0.360631

6	-1.872879	-0.002463	-0.745526
8	0.488707	-2.798254	-0.598983
8	0.477992	2.801652	-0.589863
8	-2.912865	-0.003396	-1.212859
1	2.863358	-0.870087	-1.188414
6	2.929486	0.007969	-0.541465
1	2.859446	0.889132	-1.183756
1	3.933962	0.009044	-0.101328
6	1.858509	0.002649	0.543151
1	1.980486	-0.872231	1.185472
1	1.976296	0.874669	1.190140
1	0.265774	0.002709	-1.503265
6	-0.808742	0.677200	1.975000
1	0.034945	1.230700	2.363365
1	-1.727903	1.232702	1.843784
6	-0.805400	-0.687151	1.972960
1	-1.721826	-1.246757	1.840076
1	0.041002	-1.237670	2.359660

Frequencies, cm⁻¹

43.6258	71.9867	91.0864
99.1394	112.8582	123.6067
125.7742	150.6502	173.5331
240.4324	243.1516	270.1694
400.5242	421.8985	450.0961
456.0298	456.1278	500.0323
502.5699	552.2584	596.4760
598.0518	613.4468	640.4551
721.3814	789.2965	794.4492
844.1749	951.7709	974.0564
988.3109	995.7231	1021.2019
1037.0027	1207.8593	1246.2293
1268.1092	1313.5843	1414.0140
1480.0932	1490.0626	1495.7702
1497.8904	1592.8112	1967.6563
2070.9332	2078.7191	2128.2741
2998.9465	3028.6810	3055.4608
3060.2727	3086.3457	3146.5068
3151.7401	3222.3741	3246.7544

TS3A

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.169127	-0.015933	-0.034813
6	0.883946	1.540202	-0.565507
6	-0.759376	-1.520568	-0.339324
6	1.660603	-0.853856	-0.553087
8	1.294425	2.538088	-0.942531
8	-1.372318	-2.456898	-0.571898
8	2.604152	-1.387929	-0.918448
1	-2.933334	1.080283	-1.640434

6	0.745188	0.601442	2.015791
1	0.153194	1.479809	2.237879
1	1.818407	0.738225	2.024401
6	0.198976	-0.652953	2.097224
1	0.829353	-1.529582	2.167204
1	-0.833657	-0.790797	2.389592
6	-3.023193	0.765424	-0.597600
1	-3.284142	-0.295077	-0.597722
1	-3.868993	1.309113	-0.164684
6	-1.748677	1.044628	0.200870
1	-1.521741	2.109444	0.181465
1	-1.892716	0.748416	1.239044
1	-0.818542	0.472429	-1.018807

Frequencies, cm^{-1}

-993.6160	31.6626	53.4283
94.5656	97.4649	107.0093
114.2342	129.0060	155.5104
174.6388	242.9426	259.7511
291.1012	393.6949	398.5523
446.6418	451.7297	464.0740
470.5293	499.4584	530.8285
617.8592	625.0607	645.1308
665.3474	712.8325	830.6724
841.6139	964.1227	973.1233
981.2820	984.0945	1002.3757
1032.3942	1206.6050	1242.2544
1273.4266	1298.3598	1419.4617
1466.4965	1483.7820	1498.8983
1501.4547	1583.5770	2053.7514
2056.9230	2102.3079	2113.1520
3014.8705	3052.7160	3069.5487
3081.4275	3117.3113	3140.1315
3145.7833	3213.5743	3237.5939

Table S4. Geometries and Frequencies of Species from Table2

TB_Oh

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.145177	0.023409	-0.295784
6	-0.184481	-1.580607	0.481099
6	-1.719383	0.519146	0.472792
6	1.426997	-0.338878	-1.139329
8	-0.201036	-2.603748	0.993064
8	-2.698231	0.846645	0.953022
8	2.414202	-0.547489	-1.666520
6	0.901509	1.173821	1.135629

1	1.913109	0.807544	1.257481
1	0.342967	1.236227	2.061090
6	0.574681	2.004244	0.054211
1	-0.239402	2.713106	0.136129
1	1.331241	2.284372	-0.667646
1	-0.749024	0.482749	-1.718727
1	-0.939717	-0.362242	-1.640884

Frequencies, cm^{-1}

54.7319	82.5378	96.4787
116.5594	143.9587	153.5184
331.6930	341.1422	383.4278
412.7051	447.5693	460.7987
483.5693	494.4127	494.4485
604.1230	638.2251	661.3025
695.3953	709.4680	733.7253
839.2320	939.2161	943.4309
968.1901	1007.2940	1227.2518
1233.0163	1489.1741	1555.3115
1706.2950	2067.0841	2081.4427
2135.3556	2712.6572	3128.8061
3135.9384	3193.5179	3217.8721

Cis-H₂Fe(CO)₃(η^2 -C₂H₄)

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.000123	-0.091184	-0.264460
6	-0.003262	1.617749	0.302066
6	1.751578	-0.250791	-0.619811
6	-1.750675	-0.257761	-0.620017
8	-0.005350	2.719294	0.597069
8	2.833821	-0.386467	-0.949458
8	-2.832295	-0.397479	-0.950014
6	0.000597	-0.574364	1.923477
1	-0.918707	-0.172867	2.328554
1	0.917237	-0.167416	2.329132
6	0.004292	-1.748715	1.219591
1	0.920562	-2.301604	1.065577
1	-0.908545	-2.307115	1.065059
1	0.002719	-1.355726	-1.094422
1	-0.001039	0.476021	-1.630532

Frequencies, cm^{-1}

76.1540	86.9916	94.7355
96.7916	125.9839	131.0791
266.2092	383.8866	401.9369
420.4022	441.5327	444.7597
497.6287	506.1001	549.4669
601.1876	611.7535	640.6976
715.4269	754.0771	835.4155

841.9115	844.8631	967.6910
991.6002	1006.3217	1243.2537
1302.1060	1482.0937	1586.7214
1924.5898	1966.1325	2084.0176
2089.4368	2143.1732	3144.7300
3154.4543	3218.7885	3244.7013

TS1B

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.000039	-0.101466	-0.221587
6	1.751179	-0.128960	-0.626781
6	-1.751347	-0.127242	-0.626538
6	0.000849	1.574438	0.409339
8	2.830881	-0.144197	-0.992071
8	-2.831113	-0.141407	-0.991682
8	0.001419	2.632832	0.834709
1	-0.000762	-1.575731	-0.666312
1	-0.000125	0.276472	-1.674449
6	-0.000892	-1.954872	0.903261
1	-0.908108	-2.537565	0.795697
1	0.905902	-2.538244	0.795825
6	-0.000527	-0.845765	1.766248
1	0.914405	-0.561377	2.267795
1	-0.915328	-0.560660	2.267626

Frequencies, cm⁻¹

-667.8886	71.9075	92.9864
102.0051	123.8273	132.2359
153.2773	361.9206	390.9802
443.5120	446.2270	476.6606
487.5173	495.0357	519.9407
579.3013	614.7945	662.0234
676.0517	722.8446	760.5118
842.1049	852.7236	939.6105
1067.1615	1155.8317	1243.4234
1256.7110	1481.4092	1541.6314
1895.1481	1943.8457	2079.9128
2087.0688	2140.0027	3124.2042
3144.6107	3194.0490	3230.9122

HFe(CO)₃C₂H₅-axe_q

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.000059	-0.100729	-0.212459
6	1.761013	-0.028801	-0.597880
6	-1.761006	-0.031148	-0.597798

6	-0.001015	1.528580	0.459254
8	2.846228	0.053322	-0.936259
8	-2.846344	0.049522	-0.936132
8	-0.001696	2.561930	0.946290
1	0.001181	-1.799205	-0.469801
1	-0.000060	0.083476	-1.730279
6	0.001427	-2.128710	0.683850
1	-0.895385	-2.745450	0.705375
1	0.899024	-2.744310	0.705311
6	0.000726	-0.978443	1.608614
1	0.901103	-0.830718	2.192913
1	-0.899790	-0.831894	2.192996

Frequencies, cm⁻¹

64.6537	96.8304	98.1730
122.0627	134.3852	148.2025
381.7590	390.0720	436.7231
441.7244	460.0546	482.4296
482.9390	511.7747	538.2149
539.1740	627.3434	634.0704
681.2121	685.2974	777.1561
875.7290	926.4246	1069.0912
1100.2131	1180.8827	1354.8685
1468.4169	1506.6788	1692.4659
1816.9586	2059.7893	2076.6798
2080.4835	2138.4025	3072.9297
3120.0653	3136.1039	3189.8517

TS2B

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.198226	0.065819	-0.321506
6	1.887629	-0.572784	-0.476254
6	-1.423025	0.434822	-1.072720
6	0.464925	1.518578	0.741531
8	2.927351	-0.977156	-0.720362
8	-2.337041	0.658295	-1.719429
8	0.571848	2.323427	1.546774
1	-2.094215	-0.336739	1.668143
1	-0.217418	-1.350544	-0.618480
6	-1.836842	-1.355133	1.373385
1	-2.041340	-2.007338	2.231197
1	-2.513105	-1.658814	0.570775
6	-0.384872	-1.480122	0.961190
1	-0.135899	-2.521706	0.750549
1	0.303954	-1.144853	1.738324

Frequencies, cm⁻¹

-943.4983	37.3902	61.4600
76.6668	81.3698	102.7149

113.8252	235.9173	241.6392
352.1963	370.7443	382.4567
425.2802	444.9807	458.9670
509.2246	544.4836	576.3526
595.0569	736.3172	766.7543
921.9045	989.7227	1056.2999
1211.2799	1280.2185	1406.2907
1484.1125	1485.3485	1497.0546
2010.1402	2046.0049	2052.8865
2118.3465	3004.3208	3038.6538
3063.9237	3069.5305	3101.7291

HFe(CO)₃(C₂H₅)(η^2 -C₂H₄)

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.176667	-0.000133	-0.117032
6	0.130310	1.755670	-0.335660
6	0.132205	-1.755645	-0.335319
6	-0.703946	-0.000235	1.609900
8	0.417948	2.842946	-0.524959
8	0.421007	-2.842649	-0.524408
8	-0.977844	-0.000265	2.717428
1	2.899908	0.881363	-0.985093
1	0.506345	0.000108	-1.467320
6	2.930374	0.001526	-0.338712
1	2.900854	-0.878465	-0.984924
1	3.904623	0.002097	0.166200
6	1.800985	0.001021	0.683399
1	1.878683	0.874204	1.333363
1	1.879625	-0.871941	1.333547
6	-2.404900	-0.001122	-0.461918
1	-2.781807	-0.919421	-0.031707
1	-2.782499	0.917047	-0.032034
6	-1.781095	-0.001118	-1.679357
1	-1.662796	0.913241	-2.244025
1	-1.662075	-0.915608	-2.243658

Frequencies, cm⁻¹

65.1644	76.5465	87.3960
88.2480	101.0335	111.6427
127.6225	144.1088	170.5313
242.8284	266.5356	271.2642
384.1086	402.9655	420.8397
453.3676	486.5965	502.9911
511.5053	540.8867	597.9188
613.1304	629.1819	649.0887
720.7069	781.6988	832.5876
843.5948	965.6248	973.2839
974.1985	1002.5646	1015.8293
1041.6428	1216.3768	1244.6523
1269.1677	1304.8594	1414.3457

1484.3942	1492.7663	1495.4579
1495.4761	1589.1248	1935.3454
2071.5416	2081.4783	2127.3462
2995.2543	3035.4385	3059.3050
3067.0088	3093.5500	3145.0253
3155.1498	3219.4110	3245.4478

TS3B

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.162640	-0.057574	-0.066804
6	-1.195154	-1.255525	-0.104014
6	1.364869	1.277849	-0.297026
6	0.611769	-0.385844	1.645339
8	-2.059885	-1.996355	-0.154699
8	2.088527	2.140219	-0.473883
8	0.888028	-0.580386	2.737527
1	-3.340468	2.308259	0.137578
1	-0.676921	0.767815	-0.983566
6	-2.716587	1.542010	-0.334475
1	-3.243925	0.591192	-0.235395
1	-2.658048	1.774807	-1.400634
6	-1.340161	1.512568	0.328877
1	-1.448869	1.324023	1.393854
1	-0.846617	2.475263	0.212462
6	1.562021	-1.530644	-0.775779
1	2.569024	-1.234172	-0.512070
1	1.271314	-2.510587	-0.419749
6	0.922615	-0.960475	-1.873408
1	0.131246	-1.490213	-2.386587
1	1.425014	-0.216918	-2.477616

Frequencies, cm⁻¹

-864.1744	44.9850	57.6638
74.9572	91.0835	104.9689
113.4389	133.2444	144.8723
163.0006	252.5852	275.6495
329.6581	390.8231	411.0940
426.3735	449.1667	480.3232
487.3375	501.2387	510.5460
601.0920	632.6543	653.3417
700.1230	718.4335	817.2163
839.3480	956.6683	960.4245
974.3559	980.5911	989.3206
1043.2421	1214.5757	1237.0407
1249.5393	1276.3961	1420.8550
1481.4041	1489.0118	1497.0804
1501.2042	1562.3330	2040.5800
2071.6846	2085.3227	2124.3243
3013.9261	3060.9827	3077.9195
3086.2375	3127.6956	3135.1922

3144.1813 3203.0740 3227.9823

Fe(CO)₃(C₂H₅)₂-AxEq2B

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.202121	0.000576	-0.006853
6	0.054838	1.792783	0.032004
6	0.050144	-1.791843	0.047086
6	-0.866060	0.007713	1.621435
8	0.278293	2.908926	0.086741
8	0.272583	-2.907813	0.109918
8	-1.341562	0.011272	2.661388
1	2.574678	0.871863	-1.582890
1	0.088889	-0.010167	-1.735095
6	2.766322	-0.006875	-0.960432
1	2.574475	-0.890402	-1.576039
1	3.839374	-0.006045	-0.731748
6	1.929747	-0.002183	0.317990
1	2.175629	0.868696	0.926825
1	2.174139	-0.869824	0.932007
6	-1.988206	0.003738	-0.945802
1	-2.592509	-0.886960	-0.817329
1	-2.578227	0.906472	-0.834423
6	-1.039158	-0.012877	-2.087801
1	-1.058138	0.875346	-2.717877
1	-1.063445	-0.915759	-2.696516

Frequencies, cm⁻¹

46.8676	63.3390	74.1873
98.6708	108.9927	128.1330
130.5160	150.2244	176.4254
237.4335	251.1916	366.7414
380.5468	417.8705	439.5607
467.7952	477.1961	499.3887
510.2777	515.1841	529.9563
636.8316	639.8547	651.6013
713.5694	775.8506	876.4103
944.3493	949.3199	967.3027
1024.2265	1054.3960	1104.6400
1184.6747	1198.6300	1259.1255
1371.0892	1410.5263	1466.8326
1495.0147	1498.2109	1500.2238
1508.9139	1666.9679	2067.5759
2074.4136	2127.4006	2225.2579
2991.6733	3034.9217	3052.0763
3057.1269	3067.5044	3086.9648
3114.1996	3129.1493	3179.5543

Table S5. Geometries and
Frequencies of Species from Table3

Fe(CO)₃(H₂)(η^2 -C₂H₄)

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.000076	0.008048	-0.346188
6	-1.479712	-1.006113	-0.249257
6	1.479724	-1.006198	-0.248096
6	-0.000598	0.288874	1.413548
8	-2.418602	-1.653757	-0.165784
8	2.418518	-1.653887	-0.163890
8	-0.000864	0.505689	2.533501
1	-0.403847	-0.083406	-1.979554
1	0.405134	-0.083776	-1.979265
6	0.701222	1.990596	-0.626823
1	1.248304	2.346137	0.236891
1	1.249922	2.066301	-1.557438
6	-0.700263	1.990821	-0.627360
1	-1.248231	2.066719	-1.558392
1	-1.247897	2.346517	0.235939

Frequencies, cm⁻¹

45.8693	73.2353	102.8635
105.4274	148.4136	159.1575
338.9684	346.9215	386.6679
456.5499	458.0997	464.9658
468.7218	492.0602	512.8052
533.0700	604.6779	615.5131
659.4345	688.1613	717.7856
829.9431	934.2497	944.2791
959.6265	969.0240	1228.4226
1231.3824	1483.3594	1551.2125
1645.6105	2052.8739	2070.3961
2120.5216	3129.8446	3136.0986
3194.1903	3217.9781	3404.5913

TSh2HH

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.010297	0.034167	-0.330636
6	0.071481	1.581180	0.568476
6	-1.772590	-0.106830	-0.493500
6	-0.000843	-1.259030	0.943557
8	0.106209	2.600756	1.081451
8	-2.901403	-0.191951	-0.637092
8	0.011763	-2.071708	1.745263
1	-0.018766	0.858421	-1.608176

1	-0.135671	-0.352214	-1.773025
6	1.846176	-0.888480	-1.087363
1	1.924449	-1.879226	-0.661924
1	1.853844	-0.855305	-2.167360
6	2.181356	0.231603	-0.352705
1	2.438114	1.155734	-0.851244
1	2.519709	0.136825	0.670482

Frequencies, cm^{-1}

-857.5889	61.5896	91.0112
99.7018	109.1952	127.8878
150.7223	284.8030	343.5501
408.3398	447.2284	450.2649
474.2579	500.0792	513.4337
553.2979	589.2637	629.3962
665.5521	702.9211	823.7637
840.9947	895.4389	972.2684
989.9751	1033.9984	1243.6315
1277.1358	1486.2578	1571.9272
1925.5681	2015.9326	2074.2823
2082.1724	2127.9240	3148.3012
3157.0765	3221.8161	3246.2068

Gauche-H₂Fe(CO)₃(η^2 -C₂H₄)

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.041103	-0.135652	-0.320942
6	-0.174702	1.649397	-0.146685
6	0.295337	-0.736194	1.373127
6	-1.761017	-0.498409	-0.179052
8	-0.297722	2.782745	-0.110683
8	0.489118	-1.141040	2.419709
8	-2.864748	-0.771485	-0.095870
1	2.116109	-1.813887	-0.598039
1	-0.329335	0.186484	-1.767688
6	1.884065	-0.887964	-1.105807
1	1.775872	-0.953544	-2.178251
1	-0.096514	-1.539980	-0.867309
6	2.128400	0.321937	-0.499923
1	2.218093	1.218044	-1.098547
1	2.538767	0.375469	0.499117

Frequencies, cm^{-1}

65.3468	92.1658	103.8467
107.1982	127.5216	136.4733
262.8516	320.8573	394.4854
437.8196	457.2142	465.3972
501.6523	511.6305	562.0569
583.3385	638.6098	685.3081

698.4488	723.7889	821.2226
844.3320	890.5504	990.8512
1013.0028	1027.9804	1246.5607
1291.3815	1484.1722	1578.9072
1888.4574	1929.4776	2087.4108
2089.9864	2139.6803	3149.6173
3160.2696	3226.5135	3253.2114

TS1C/D (Geometry at BP86/lanl2dz)

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.007634	0.020293	-0.358375
6	0.098802	1.538006	0.565415
6	-0.040283	-1.252212	0.922261
6	-1.738082	-0.046145	-0.536912
8	0.143379	2.591682	1.118258
8	-0.101354	-2.091638	1.764333
8	-2.920317	-0.104955	-0.654896
1	1.895986	-1.823698	-1.130007
1	0.030181	0.995320	-1.534947
6	1.845458	-0.735399	-1.238819
1	1.952069	-0.354356	-2.258490
1	-0.058568	-0.949441	-1.539649
6	2.174687	0.103180	-0.136648
1	2.520932	1.124235	-0.325892
1	2.443761	-0.324969	0.833385

Frequencies, cm^{-1}

-88.5814	151.8613	162.0757
191.7662	194.7140	244.3236
269.6651	389.6206	438.9317
471.3696	514.8273	530.4348
558.5691	579.1213	649.3873
666.9502	681.7439	718.9310
752.0545	802.7261	839.5197
887.9230	906.8637	1028.5535
1040.0472	1101.9745	1163.4532
1257.3696	1491.4969	1542.2225
1719.2357	1743.5780	1801.9377
1839.9125	1864.0898	3033.7481
3035.9238	3108.8868	3131.1872

HFe(CO)₃C₂H₅-eqeq

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.032303	-0.107972	-0.361367
6	-0.207581	1.589840	0.026567

6	0.351942	-0.810144	1.291305
6	-1.775076	-0.504337	-0.153314
8	-0.285340	2.713905	0.214881
8	0.573554	-1.206099	2.335003
8	-2.885583	-0.632713	0.075171
1	2.334403	-1.790468	-0.883502
1	-0.383147	0.489240	-1.713872
6	1.774870	-0.959866	-1.311350
1	1.924738	-0.902615	-2.386660
1	0.664926	-1.398639	-1.271658
6	1.925243	0.333942	-0.593086
1	2.134494	1.193483	-1.217666
1	2.527035	0.318927	0.307737

Frequencies, cm^{-1}

76.0057	89.8365	104.4148
129.3060	136.1218	153.6046
353.8176	361.8709	422.7580
447.3886	465.9696	491.7292
502.3397	519.9160	548.7714
585.9727	614.2968	627.2050
784.0389	828.3767	855.4045
880.2630	971.4161	1049.1334
1117.9494	1174.9923	1348.0380
1467.3739	1504.5510	1688.7643
1869.6346	2075.2762	2083.8175
2105.6588	2137.5711	3076.0213
3120.5637	3143.1027	3193.4428

TS2C

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.073525	-0.144695	-0.072698
6	-1.064707	0.920279	-0.900941
6	0.440099	1.150708	1.150628
6	-1.138576	-1.320400	0.534201
8	-1.791297	1.592437	-1.473532
8	0.622744	1.971079	1.927241
8	-1.929380	-2.063565	0.897051
1	2.923260	-0.463672	0.387699
1	0.191919	-0.816871	-1.426161
6	2.148574	-1.011765	-0.142333
1	2.447612	-2.046475	-0.308319
1	1.320954	-1.172924	0.661669
6	1.649005	-0.322379	-1.375021
1	1.743445	-0.911498	-2.283995
1	2.038250	0.675235	-1.546028

Frequencies, cm^{-1}

-938.2470	66.7299	84.5601
-----------	---------	---------

97.8706	112.1163	128.8619
145.0422	335.3517	357.4142
415.8292	447.6995	467.0938
468.6655	500.5686	512.1869
532.6803	583.7574	613.5587
634.4073	746.2220	874.8553
994.4935	1038.5978	1087.9838
1153.6992	1192.7562	1363.7369
1465.3546	1512.7285	1659.4555
1991.0959	2055.3213	2056.8533
2114.8644	2342.4837	3073.7942
3092.8186	3141.4649	3159.5497

HFe(CO)₃(C₂H₅)(η^2 -C₂H₄)

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.210080	0.016150	-0.208680
6	-0.687696	1.697826	-0.452337
6	0.231577	0.163478	1.533842
6	-1.939015	-0.524818	-0.068077
8	-0.990871	2.780777	-0.642875
8	0.545282	0.300081	2.622139
8	-3.032919	-0.836878	-0.000862
1	2.958878	-0.165143	1.025819
1	-0.368966	0.055456	-1.714365
6	2.946492	-0.075441	-0.064020
1	3.893866	0.396116	-0.351640
1	2.972595	-1.087182	-0.477507
6	1.766850	0.751119	-0.571195
1	1.820605	0.853969	-1.655152
1	1.845131	1.757754	-0.155632
6	0.366126	-1.851210	-1.252151
1	-0.467876	-2.182147	-1.855285
1	1.275120	-1.629168	-1.792049
6	0.392603	-2.105232	0.098896
1	1.326840	-2.088576	0.640884
1	-0.427670	-2.617161	0.583639

Frequencies, cm^{-1}

68.2528	87.6769	92.6808
95.6690	105.1678	122.7556
147.6753	181.2112	203.2017
238.7292	283.4339	287.9226
386.5891	421.5403	441.0868
465.6156	468.4532	484.7733
516.1686	522.7969	576.7591
593.6315	639.9289	686.0467
697.4028	736.8364	793.0278
842.3882	962.9755	982.5129
986.7378	1003.1320	1016.5898
1032.7135	1207.8785	1244.8852

1284.1147	1289.7389	1410.5723
1476.1174	1485.4302	1503.7207
1505.6794	1577.7320	1915.2193
2078.6259	2082.7138	2129.6421
2999.1895	3032.0139	3048.6284
3062.9333	3091.6200	3152.5250
3158.7697	3229.9107	3250.9281

HFe(CO)₃(C₂H₅)₂-AxEq2C

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.232384	-0.024941	-0.104878
6	-0.826316	1.542650	-0.778147
6	0.284214	0.451591	1.503354
6	-1.875295	-0.672564	0.332144
8	-1.169027	2.544252	-1.201382
8	0.683047	0.731722	2.537406
8	-2.891879	-1.085319	0.639520
1	3.052964	-0.005158	0.868226
1	-0.238383	-0.795161	-1.674363
6	2.958945	0.053663	-0.219251
1	3.836089	0.599956	-0.586078
1	3.043031	-0.961689	-0.613267
6	1.680892	0.761285	-0.656553
1	1.612913	0.773324	-1.748357
1	1.730336	1.804690	-0.340553
6	0.264767	-1.810927	-1.352266
1	-0.464153	-2.521878	-1.740167
1	1.167614	-1.803800	-1.960556
6	0.499107	-1.895757	0.110656
1	1.529962	-1.942430	0.431605
1	-0.123405	-2.604277	0.646354

Frequencies, cm⁻¹

78.4443	80.8658	87.3979
99.8061	101.4754	124.4339
141.1312	190.9473	231.3452
255.1458	310.2005	358.4564
413.4399	429.1060	459.1368
471.0745	483.7310	489.4917
512.9262	523.4729	544.2622
602.4828	613.8587	630.7980
698.4276	802.1547	879.1183
957.0936	964.1398	985.0531
1018.1945	1057.3776	1113.2738
1177.4449	1208.3650	1283.2277
1364.6124	1411.4531	1462.3066
1482.1027	1494.9231	1497.9001
1522.1178	1662.7737	2068.7422
2077.5585	2128.0592	2235.2880
3001.3144	3019.2316	3050.5649

3061.7804	3067.1955	3085.9983
3120.3467	3133.8885	3206.6345

TS3C

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.201970	-0.011717	-0.070786
6	-0.885772	1.514582	-0.735036
6	0.263323	0.338081	1.619752
6	-1.865436	-0.617346	0.254605
8	-1.299637	2.493001	-1.154964
8	0.607214	0.542093	2.690576
8	-2.914146	-1.014839	0.466445
1	3.043969	-0.190109	0.749530
1	0.660584	-0.152075	-1.343194
6	3.006116	-0.000582	-0.324489
1	3.911559	0.554767	-0.592527
1	3.070821	-0.965835	-0.832743
6	1.768395	0.791836	-0.721345
1	1.834454	1.084785	-1.775055
1	1.712787	1.727363	-0.170446
6	0.277882	-1.638555	-1.343163
1	-0.614684	-1.961307	-1.863723
1	1.152290	-1.666616	-1.991980
6	0.458276	-1.982193	0.035131
1	1.462993	-2.094917	0.419276
1	-0.267711	-2.628384	0.512100

Frequencies, cm⁻¹

-1295.1303	70.1876	80.6633
87.2299	100.1491	102.8589
123.4388	155.6519	210.5785
226.2939	263.7933	276.3433
380.1499	418.0395	432.0617
466.0238	478.3931	480.7280
505.4374	520.0889	536.6849
590.7990	621.3540	634.7326
675.5824	748.3988	804.4005
837.8420	946.0028	974.5064
990.9415	1015.3459	1048.4777
1127.8289	1193.9958	1226.4229
1246.5541	1292.6634	1418.8555
1478.2424	1486.3442	1500.2352
1505.3244	1528.5579	2003.8072
2059.9103	2064.9634	2118.8270
3010.5427	3015.8951	3060.4010
3084.0959	3090.4077	3111.0668
3136.8868	3179.2217	3216.3878

Table S6. Geometries and
Frequencies of Species from Table4

TSrotD

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.181815	0.021807	-0.389557
6	-0.397785	1.373384	0.666831
6	0.408370	-1.186643	0.866910
6	-1.921656	-0.527955	-0.515408
8	-0.506957	2.307566	1.316392
8	0.715018	-1.870000	1.723205
8	-3.023227	-0.789981	-0.627641
1	3.037015	-0.603077	0.254880
1	-0.652647	1.111708	-1.331976
6	2.743693	-0.350714	-0.766880
1	3.650497	-0.025471	-1.292758
1	2.422234	-1.275970	-1.257667
6	1.675602	0.739695	-0.809352
1	1.501419	1.070280	-1.839399
1	2.003120	1.620483	-0.256863

Frequencies, cm⁻¹

-123.6729	75.8456	83.7988
101.4074	103.5995	120.5841
205.8876	269.8365	329.2633
417.3818	430.1504	436.7236
472.5252	497.0595	509.7402
543.6469	568.8979	595.9618
652.4388	763.5078	830.4766
943.5405	968.0786	1009.7606
1184.4872	1257.6062	1406.8201
1456.8713	1489.6854	1498.7488
1878.7191	2074.6068	2092.2043
2141.8498	2988.0997	3006.0328
3027.2970	3069.1735	3087.0745

HFe(CO)₃C₂H₅-W

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.203967	-0.075053	-0.380936
6	0.170430	-1.298057	0.851283
6	-0.249165	1.366975	0.661071
6	1.999599	0.222645	-0.481065
8	0.100412	-2.148409	1.612121
8	-0.488271	2.222730	1.372185
8	3.128069	0.331077	-0.585417

1	-3.287265	-0.462600	0.245482
1	0.582150	-1.313783	-1.167392
6	-2.887271	0.162239	-0.558508
1	-3.646280	0.173416	-1.349901
1	-2.794085	1.179214	-0.173770
6	-1.577488	-0.410304	-1.054855
1	-1.086817	0.257621	-1.839238
1	-1.729152	-1.386655	-1.509512

Frequencies, cm⁻¹

52.9396	80.2995	84.3434
100.1213	106.2963	154.4286
230.7372	266.6444	369.2224
396.0629	427.4741	442.5051
487.3946	522.5182	528.0579
578.0918	581.4944	610.2094
659.9885	794.0060	857.8430
903.6176	985.6520	1039.0364
1183.5282	1222.1420	1409.5266
1409.5989	1484.5743	1494.9030
1890.2597	2073.1560	2091.0092
2140.4825	2589.5504	3002.4014
3052.4221	3084.1056	3112.8258

TS2D

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.173520	-0.064424	-0.333826
6	0.315331	-0.661520	1.305609
6	-0.343227	1.613330	0.195841
6	1.960919	-0.135840	-0.612517
8	0.367043	-1.087842	2.365452
8	-0.623491	2.649154	0.587513
8	3.083738	-0.211715	-0.810996
1	-2.924711	-1.190061	0.517139
1	-0.139681	-1.478566	-0.719150
6	-2.831487	-0.583950	-0.386711
1	-3.693637	-0.821739	-1.020497
1	-2.898360	0.461831	-0.087749
6	-1.522954	-0.898042	-1.107421
1	-1.335137	-0.206890	-1.958952
1	-1.609805	-1.890204	-1.555878

Frequencies, cm⁻¹

-888.8067	36.8872	69.4924
76.1850	96.8452	101.6515
145.4472	219.3804	258.6343
304.7369	364.8338	415.6309
435.3369	459.9135	479.5801
516.7330	551.9867	567.7436

617.7795	715.1066	776.2664
920.5478	1004.3253	1082.5376
1209.4915	1329.4194	1411.0543
1433.9364	1491.3734	1497.7847
2028.3811	2056.4385	2075.1385
2119.6996	2851.8333	3005.6018
3043.9767	3069.6858	3108.8913

HFe(CO)₃(C₂H₅)₂-AxEq2D

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	-0.236577	0.037317	-0.082643
6	0.533756	1.613924	-0.497860
6	0.365742	-0.290498	1.533113
6	-1.830678	0.747036	0.432059
8	1.045130	2.597456	-0.766480
8	0.760260	-0.575440	2.567334
8	-2.810953	1.194531	0.802954
1	3.118272	0.772571	-0.315263
1	-0.762566	-0.219171	-1.729258
6	2.958744	-0.292108	-0.128467
1	3.796619	-0.824323	-0.593708
1	3.043044	-0.450913	0.949271
6	1.629307	-0.792610	-0.686515
1	1.530866	-1.862970	-0.499699
1	1.607401	-0.640471	-1.769134
6	-1.150199	-1.324444	-1.596659
1	-2.165363	-1.227306	-1.979436
1	-0.510251	-1.853507	-2.300895
6	-1.057201	-1.801472	-0.193762
1	-0.357970	-2.609051	-0.011844
1	-2.001430	-1.954531	0.317403

Frequencies, cm⁻¹

68.3966	77.2046	81.7122
98.5944	101.4815	120.9335
129.8809	175.7749	226.1379
251.4657	273.9987	358.3321
413.2158	435.3193	461.3702
483.7543	485.2545	492.9686
514.9907	531.3875	546.1155
599.7257	616.5867	644.1722
698.5262	807.8552	883.2775
956.1934	960.1717	985.8636
1023.6598	1056.9882	1114.7492
1178.1463	1201.1664	1276.1035
1370.6276	1419.1094	1461.0214
1477.4759	1500.3609	1503.4982
1507.2967	1668.6992	2068.2139
2075.3397	2126.8818	2234.4462
3003.7915	3020.8956	3056.0966

3068.4958	3068.9151	3091.7517
3112.2252	3133.8063	3183.0678

TS3D

Charge = 0 Multiplicity = 1

Cartesian Coordinates

26	0.159266	0.072644	-0.137888
6	-0.596697	-1.391642	-0.797304
6	0.273683	-0.318043	1.614624
6	1.754002	-0.533436	-0.719475
8	-1.089310	-2.323789	-1.238399
8	0.287447	-0.547804	2.733537
8	2.771463	-0.904121	-1.083010
1	-3.239553	-0.425541	-0.609264
6	-2.994504	0.027121	0.354299
1	-3.886212	0.566503	0.692226
1	-2.817391	-0.784767	1.062508
6	-1.806561	0.974367	0.262332
1	-1.592135	1.416284	1.232723
1	-2.049005	1.811429	-0.397912
6	0.772579	1.989006	-0.983100
1	1.566239	1.838514	-1.702323
1	-0.090987	2.510956	-1.370832
6	1.038578	1.993155	0.378511
1	0.376008	2.503499	1.064521
1	2.046079	1.830382	0.738336
1	-0.857224	0.606548	-1.081245

Frequencies, cm⁻¹

-972.9752	43.4126	62.4260
87.6724	100.1195	108.2555
124.9159	145.7525	178.3117
192.2479	258.0212	261.5544
298.6108	407.4798	425.6461
453.2408	472.3553	483.6296
493.2767	514.5764	529.4841
573.6954	624.6305	630.0972
687.7562	747.2909	780.1776
837.2880	960.0110	980.4996
984.5057	995.2910	1022.7132
1067.5796	1225.5308	1241.7018
1261.6554	1281.1826	1418.6642
1484.8535	1496.5591	1498.5252
1503.2044	1563.6094	2055.5030
2061.5184	2086.9511	2119.1490
3010.8797	3030.2048	3063.9063
3083.6724	3106.1557	3140.7180
3150.0276	3212.8114	3236.5512

Full Citation for Ref. [84]

Gaussian 03, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.