

The Infrared Dynamics of Iron Diene Complexes.

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Computational Details

Geometries were fully optimised at the BP86/AE1 level, i.e. employing the exchange and correlation functionals of Becke¹ and Perdew,² respectively, together with an ultrafine integration grid (a pruned grid with 99 radial shells with 590 angular points per shell) and the augmented Wachters' basis³ on Fe (8s7p4d) and 6-31G(d) basis elsewhere. Tight optimization convergence criteria were applied throughout. Starting from the transition states, the intrinsic reaction coordinate (IRC)⁴ was followed in internal (Z-Matrix) coordinates until (or close to) the respective minima (due to symmetry, only one such path needs to be followed in each case), again using tight convergence criteria. Harmonic frequencies were computed analytically for the stationary points (minima and transition states) as well as for selected points on the IRCs, and are reported without scaling (See Tables S1 and S2). In addition, the stationary points and the IRC were recomputed for the COD complex at the BP86/ECP2 level, i.e. using a relativistically adjusted pseudopotential on Fe (denoted SDD)⁵ along with its (6s5p3d1f) valence basis and 6-311+G(d,p) basis elsewhere, again using the ultrafine grid and tight convergence criteria (see results in Table S3). All computations employed the Gaussian 03 program package.⁶

Table S1: CO stretching frequencies (cm^{-1}) in NBD, calculated at the BP86/AE1 level along the IRC (value for the coordinate given in $\text{amu}^{1/2}$ Bohr, relative energies in kcal mol^{-1}).

IRC	E_{rel}	a''	a'	a'	$\Delta(\text{a}''-\text{a}')^a$
Ground state	0.0	1971	1982	2026	11
0.56	0.01	1971	1982	2026	11
0.48	0.04	1971	1982	2027	11
0.40	0.12	1971	1982	2027	11
0.32	0.22	1971	1982	2027	11
0.24	0.33	1971	1981	2027	10
0.16	0.43	1971	1981	2027	10
0.08	0.51	1971	1981	2027	10
Transition state	0.53	1971	1981	2027	10

^a Separation of the two low frequency modes (labels according to modes in C_s symmetry).

Table S2: CO stretching frequencies (cm^{-1}) in COD, calculated at the BP86/AE1 level along the IRC (value for the coordinate given in $\text{amu}^{1/2}$ Bohr, relative energies in kcal mol^{-1}).

IRC	E_{rel}	a''	a'	a'	$\Delta(\text{a}''-\text{a}')^a$
Ground state	0.0	1964	1977	2020	13
0.48	0.09	1965	1976	2019	11
0.40	0.16	1964	1976	2019	12
0.32	0.24	1964	1976	2019	12
0.24	0.31	1963	1976	2020	13
0.16	0.38	1963	1976	2020	13
0.08	0.41	1962	1976	2020	14
Transition state	0.42	1962	1976	2021	14

^a Separation of the two low frequency modes (using the same labels as in Table S1).

Table S3: CO stretching frequencies (cm^{-1}) in COD, calculated at the BP86/ECP2 level along the IRC (value for the coordinate given in $\text{amu}^{1/2}$ Bohr, relative energies in kcal mol^{-1}).

IRC	E_{rel}	a''	a'	a'	$\Delta(a''-a')^a$
Ground state	0.0	1944	1957	2007	13
0.68	0.00	1944	1957	2007	13
0.56	0.03	1945	1957	2006	12
0.44	0.09	1945	1957	2006	12
0.32	0.18	1944	1957	2006	13
0.20	0.26	1943	1957	2007	14
0.08	0.31	1942	1957	2007	15
Transition state	0.31	1941	1957	2008	16

^a Separation of the two low frequency modes (using the same labels as in Table S1).

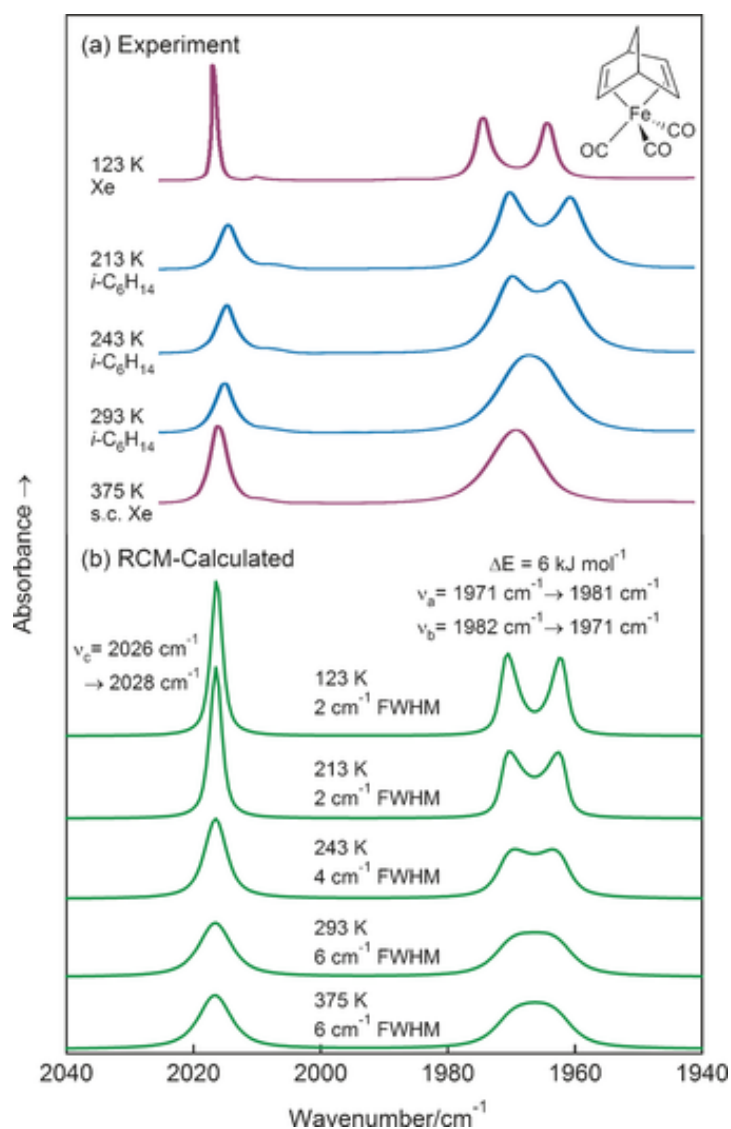


Figure S1. (Fig. 6 taken from reference 7) “(a) Experimental and (b) RCM-calculated C-O IR spectra of (norbornadiene)Fe(CO)₃. The calculated spectra use the DFT-calculated spectra for the ground and transition states from reference 8 and the experimental spectra are redrawn from the spectra presented by Turner et al⁹ and Giordano and Lear¹⁰ and were obtained either as matrix-isolated samples in Xe or as solutions in 2-methylpentane(*i*-C₆H₁₄) or supercritical Xe.” (Note that, as stated in the main text, the calculation assumes that the two low frequency bands swap over in climbing the potential well; which we believe is incorrect). Reprinted with permission from John Wiley & Sons.

References

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BP86 optimised coordinates of stationary points
and points on IRC paths used for harmonic
frequency calculations (xyz coordinates in
Ångstrom).

NOR minimum //BP86/AE1

26	0.006254	0.512103	0.000000
6	-0.818005	-1.098651	1.163123
6	0.599629	-1.163354	1.180558
6	0.599629	-1.163354	-1.180558
6	-0.818005	-1.098651	-1.163123
6	-0.191855	-3.100386	0.000000
6	-1.283371	-1.994250	0.000000
6	0.988553	-2.086455	0.000000
1	-1.462592	-0.783630	1.986067
1	1.244874	-0.929889	2.029854
1	1.244874	-0.929889	-2.029854
1	-1.462592	-0.783630	-1.986067
1	-0.219121	-3.733052	0.907128
1	-0.219121	-3.733052	-0.907128
1	-2.340802	-2.292387	0.000000
1	2.016257	-2.475789	0.000000
6	1.717522	1.049300	0.000000
6	-0.688781	1.570132	-1.253936
6	-0.688781	1.570132	1.253936
8	2.829383	1.413730	0.000000
8	-1.131165	2.258126	-2.093150
8	-1.131165	2.258126	2.093150

NBD IRC 0.56 //BP86/AE1

26	0.512120	0.004244	-0.004621
6	-3.100642	-0.186521	0.031654
1	-3.722771	-0.176786	0.946331
1	-3.743391	-0.252809	-0.866380
6	-1.996054	-1.279416	0.068688
6	-2.084969	0.990494	-0.030426
6	-1.088400	-0.765797	1.201821
6	-1.150588	0.652696	1.156785
6	-1.111248	-0.867055	-1.122153
6	-1.174493	0.547167	-1.201833
1	-2.296138	-2.335188	0.117164
1	-2.472369	2.018035	-0.073219
1	-0.771120	-1.374107	2.051117
1	-0.912610	1.334342	1.975917
1	-0.800202	-1.547638	-1.917114
1	-0.943555	1.154114	-2.079532
6	1.580766	-0.575594	1.296659
6	1.557916	-0.799952	-1.203753
6	1.051366	1.709873	-0.134699
8	2.272382	-0.941048	2.169019
8	2.241101	-1.313104	-2.006005
8	1.417155	2.818441	-0.214341

NBD IRC 0.48 //BP86/AE1

26	0.511900	0.000747	-0.010665
6	-3.101152	-0.170774	0.074651
1	-3.708995	-0.107796	0.996693
1	-3.757594	-0.289748	-0.808006
6	-1.999744	-1.264372	0.164029
6	-2.082323	0.995489	-0.073860
6	-1.075204	-0.686712	1.252069
6	-1.132567	0.728261	1.118692
6	-1.130289	-0.929570	-1.061803
6	-1.190180	0.475256	-1.227864
1	-2.303318	-2.313873	0.280096
1	-2.466208	2.020098	-0.176502
1	-0.756429	-1.241937	2.136500
1	-0.886923	1.458772	1.892251
1	-0.825480	-1.658698	-1.814987
1	-0.961251	1.026817	-2.141824
6	1.593337	-0.413137	1.340673
6	1.537589	-0.953033	-1.116018
6	1.060561	1.679409	-0.323249
8	2.288696	-0.668262	2.248225
8	2.212466	-1.563410	-1.854999
8	1.433418	2.771926	-0.514582

NBD IRC 0.40 //BP86/AE1

26	0.511398	-0.001833	-0.015996
6	-3.102025	-0.148365	0.113318
1	-3.696254	-0.048777	1.040894
1	-3.771615	-0.298767	-0.754655
6	-2.004366	-1.243273	0.231438
6	-2.080018	1.005732	-0.095225
6	-1.062676	-0.628441	1.284363
6	-1.114556	0.781846	1.093074
6	-1.151422	-0.961255	-1.019180
6	-1.207022	0.434085	-1.239421
1	-2.311575	-2.285917	0.391534
1	-2.460219	2.027345	-0.234692
1	-0.742619	-1.148144	2.189741
1	-0.859614	1.542649	1.833812
1	-0.854579	-1.720220	-1.745575
1	-0.979411	0.949203	-2.174667
6	1.605553	-0.270750	1.359742
6	1.510128	-1.084930	-1.024971
6	1.078590	1.634255	-0.482651
8	2.305269	-0.431114	2.285062
8	2.172412	-1.780186	-1.697658
8	1.465622	2.700908	-0.769081

NBD IRC 0.32 //BP86/AE1

26	0.510707	-0.003457	-0.020408
6	-3.103295	-0.121305	0.143224
1	-3.685369	-0.011754	1.077273
1	-3.784620	-0.273327	-0.715385
6	-2.011016	-1.222292	0.256441
6	-2.076586	1.024702	-0.086205
6	-1.052970	-0.606450	1.294619
6	-1.097254	0.803884	1.090498
6	-1.173481	-0.954349	-1.008097
6	-1.222429	0.437753	-1.236287
1	-2.323201	-2.261918	0.426385
1	-2.451699	2.047617	-0.229681
1	-0.732730	-1.119797	2.203620
1	-0.831715	1.570248	1.821784
1	-0.886070	-1.719070	-1.732231
1	-0.994446	0.946428	-2.174922
6	1.615269	-0.168862	1.361780
6	1.476159	-1.185057	-0.950655
6	1.106871	1.587470	-0.594078
8	2.318341	-0.263265	2.293208
8	2.121552	-1.945237	-1.567371
8	1.515590	2.625815	-0.947547

NBD IRC 0.24 //BP86/AE1

26	0.509923	-0.003755	-0.023852
6	-3.104697	-0.091820	0.165209
1	-3.676604	0.006103	1.106728
1	-3.795816	-0.221957	-0.689243
6	-2.019415	-1.202641	0.246709
6	-2.071669	1.050925	-0.052765
6	-1.046618	-0.614180	1.287917
6	-1.081391	0.801015	1.107903
6	-1.195050	-0.916214	-1.023260
6	-1.234615	0.478711	-1.221678
1	-2.337940	-2.243130	0.398832
1	-2.440284	2.079053	-0.173884
1	-0.727521	-1.145315	2.187108
1	-0.804761	1.553312	1.849656
1	-0.918183	-1.667241	-1.765600
1	-1.004586	1.005686	-2.149636
6	1.622607	-0.101276	1.357036
6	1.435343	-1.262116	-0.894735
6	1.144977	1.544067	-0.668356
8	2.328344	-0.154226	2.289344
8	2.058695	-2.073462	-1.467384
8	1.581819	2.554225	-1.067921

NBD IRC 0.16 //BP86/AE1

26	0.509253	-0.003000	-0.026260
6	-3.105850	-0.061615	0.180464
1	-3.670030	0.010066	1.128927
1	-3.804386	-0.154591	-0.672880
6	-2.028832	-1.183126	0.213118
6	-2.065172	1.080273	-0.003471
6	-1.043658	-0.641165	1.268863
6	-1.067606	0.780650	1.138020
6	-1.214287	-0.856320	-1.054510
6	-1.242116	0.543992	-1.197767
1	-2.354912	-2.225988	0.328858
1	-2.426110	2.114984	-0.084897
1	-0.727292	-1.205603	2.148571
1	-0.780308	1.505080	1.903113
1	-0.948097	-1.579685	-1.827594
1	-1.008375	1.105063	-2.104568
6	1.628020	-0.057047	1.351200
6	1.389495	-1.323616	-0.853046
6	1.189493	1.503900	-0.718678
8	2.335992	-0.085083	2.282582
8	1.986452	-2.177094	-1.391360
8	1.657806	2.486317	-1.151463

NBD IRC 0.08 //BP86/AE1

26	0.508778	-0.001635	-0.027665
6	-3.106613	-0.030843	0.189308
1	-3.666015	0.006706	1.142518
1	-3.809735	-0.078810	-0.664040
6	-2.038753	-1.161523	0.165324
6	-2.057226	1.109670	0.052985
6	-1.044489	-0.676960	1.241366
6	-1.056647	0.750029	1.173339
6	-1.229518	-0.783002	-1.092562
6	-1.243764	0.621801	-1.166820
1	-2.373354	-2.205843	0.234527
1	-2.409581	2.149975	0.020079
1	-0.732790	-1.282077	2.095362
1	-0.759675	1.438104	1.967739
1	-0.973524	-1.469883	-1.901529
1	-1.004256	1.224370	-2.045050
6	1.631035	-0.025854	1.347261
6	1.340274	-1.375636	-0.819274
6	1.238508	1.463888	-0.756210
8	2.340270	-0.038045	2.277822
8	1.907480	-2.265754	-1.329247
8	1.740232	2.417619	-1.215901

NOR TS //BP86/AE1

26	-0.508566	0.000000	-0.028108
6	3.106919	-0.000003	0.192005
1	3.664781	-0.000005	1.146840
1	3.811524	-0.000005	-0.661489
6	2.048373	1.137018	0.110402
6	2.048370	-1.137021	0.110405
6	1.049036	0.714431	1.208694
6	1.049034	-0.714429	1.208695
6	1.239422	0.703236	-1.131118
6	1.239420	-0.703241	-1.131116
1	2.391841	2.180617	0.128854
1	2.391835	-2.180621	0.128860
1	0.743870	1.361838	2.033569
1	0.743868	-1.361834	2.033572
1	0.992415	1.348861	-1.976050
1	0.992411	-1.348867	-1.976046
6	-1.631789	-0.000005	1.346082
6	-1.289560	1.421627	-0.788225
6	-1.289565	-1.421618	-0.788234
8	-2.341299	-0.000008	2.276444
8	-1.824834	2.344746	-1.272768
8	-1.824842	-2.344733	-1.272782

BUT minimum //BP86/AE1

26	0.008002	0.007897	0.000000
6	1.000284	-1.675234	0.713067
6	1.000284	-1.675234	-0.713067
6	-0.271885	-1.593742	1.372758
6	-0.271885	-1.593742	-1.372758
1	1.944873	-1.585836	1.261391
1	1.944873	-1.585836	-1.261391
1	-0.279495	-1.390901	2.449117
1	-0.279495	-1.390901	-2.449117
1	-1.114994	-2.201709	1.027298
1	-1.114994	-2.201709	-1.027298
6	-1.734690	0.393643	0.000000
6	0.617679	1.098044	1.280799
6	0.617679	1.098044	-1.280799
8	-2.882272	0.612005	0.000000
8	1.000284	1.809054	2.126485
8	1.000284	1.809054	-2.126485

BUT IRC 1.20 //BP86/AE1

26	-0.001369	-0.015063	0.035799
6	-1.312473	-1.023174	-1.303462
6	-1.891128	0.723789	0.750423
6	-1.242043	0.380251	-1.586546
6	-1.540224	1.279751	-0.519817
1	-0.836309	0.765002	-2.528842
1	-1.355437	2.352808	-0.645929
1	-0.907566	-1.718514	-2.046682
1	-1.914426	1.390387	1.618621
1	-2.146784	-1.431358	-0.722427
1	-2.565397	-0.135733	0.8217988
6	0.984897	1.335593	0.681783
6	0.012247	-1.272884	1.304193
6	1.382333	-0.537578	-0.960045
8	1.648430	2.227880	1.044218
8	0.004802	-2.098369	2.131194
8	2.271750	-0.897691	-1.628246

BUT IRC 1.00 //BP86/AE1

26	-0.009483	0.035588	-0.042960
6	-1.162926	0.472873	1.701316
6	-1.999972	-0.288403	-0.817633
6	-1.165667	-0.926070	1.398320
6	-1.598405	-1.312089	0.093458
1	-0.727027	-1.670405	2.071927
1	-1.482893	-2.352586	-0.231315
1	-0.668552	0.799986	2.622362
1	-2.133700	-0.555591	-1.870794
1	-1.999508	1.111301	1.396870
1	-2.603771	0.559374	-0.480162
6	0.904068	-1.093123	-1.097723
6	0.008321	1.637942	-0.831217
6	1.435426	0.195742	0.982937
8	1.540188	-1.866676	-1.702267
8	0.014151	2.683501	-1.353854
8	2.362779	0.315851	1.685034

BUT IRC 0.80 //BP86/AE1

26	-0.013698	0.048315	-0.039065
6	-1.044084	0.013827	1.844124
6	-2.070391	0.153245	-0.716889
6	-1.198045	-1.212354	1.125657
6	-1.730088	-1.131114	-0.198939
1	-0.810563	-2.164427	1.503914
1	-1.740845	-2.022078	-0.837004
1	-0.484667	-0.006418	2.785500
1	-2.290003	0.238227	-1.786004
1	-1.817879	0.788208	1.805725
1	-2.554051	0.906078	-0.087717
6	0.808446	-0.914434	-1.312312
6	0.117676	1.772211	-0.476849
6	1.454862	-0.068445	0.951578
8	1.397188	-1.597672	-2.057756
8	0.205387	2.896455	-0.787320
8	2.400413	-0.132957	1.636705

BUT IRC 0.60 //BP86/AE1

26	0.012308	0.051716	0.024692
6	0.991975	-0.483338	-1.820826
6	2.055831	0.644382	0.464755
6	1.336002	-1.362924	-0.749442
6	1.888761	-0.770032	0.431560
1	1.083070	-2.428280	-0.763839
1	2.049877	-1.381043	1.326617
1	0.422476	-0.893812	-2.661309
1	2.300868	1.112434	1.423699
1	1.639051	0.357613	-2.092381
1	2.397194	1.196227	-0.415734
6	-0.698494	-0.704950	1.489071
6	-0.324187	1.796477	0.115831
6	-1.434990	-0.375636	-0.903511
8	-1.214770	-1.261947	2.379358
8	-0.549297	2.941121	0.212809
8	-2.373675	-0.650627	-1.545126

BUT IRC 0.40 //BP86/AE1

26	0.007042	0.042991	0.007248
6	1.039017	-0.956651	-1.611142
6	1.930370	1.055599	0.054900
6	1.536738	-1.335166	-0.327827
6	2.000635	-0.284109	0.532655
1	1.466322	-2.362396	0.044553
1	2.277741	-0.504217	1.569234
1	0.537552	-1.721806	-2.212805
1	2.114765	1.865855	0.767907
1	1.525534	-0.173294	-2.201900
1	2.158387	1.301641	-0.986280
6	-0.596245	-0.450350	1.623085
6	-0.572817	1.704782	-0.217848
6	-1.368004	-0.701049	-0.820366
8	-1.034536	-0.827859	2.640313
8	-0.958057	2.805810	-0.326764
8	-2.267600	-1.193188	-1.384787

BUT IRC 0.20 //BP86/AE1

26	0.001357	0.024041	-0.004547
6	1.196804	-1.269295	-1.270063
6	1.710134	1.302746	-0.414715
6	1.753063	-1.106943	0.033802
6	2.020429	0.234877	0.475631
1	1.868562	-1.948947	0.724012
1	2.336132	0.423138	1.507160
1	0.840960	-2.265110	-1.553852
1	1.749838	2.324378	-0.022756
1	1.527803	-0.653835	-2.112929
1	1.892219	1.220427	-1.490510
6	-0.524456	-0.210084	1.693688
6	-0.826752	1.522719	-0.454140
6	-1.244814	-1.006525	-0.718239
8	-0.903192	-0.394880	2.785303
8	-1.375515	2.523694	-0.720112
8	-2.065947	-1.695075	-1.191276

BUT TS //BP86/AE1

26	0.001074	0.000000	-0.008510
6	-1.441193	1.379028	-0.864425
6	-1.441190	-1.379028	-0.864430
6	-1.931569	0.719378	0.300586
6	-1.931569	-0.719382	0.300584
1	-2.189505	1.271247	1.210374
1	-2.189503	-1.271255	1.210370
1	-1.282566	2.461060	-0.810480
1	-1.282562	-2.461060	-0.810489
1	-1.660562	1.003588	-1.868921
1	-1.660559	-1.003585	-1.868925
6	0.497646	-0.000003	1.714201
6	1.060238	-1.283741	-0.604996
6	1.060235	1.283746	-0.604991
8	0.853351	-0.000005	2.828918
8	1.760936	-2.143758	-0.983202
8	1.760932	2.143766	-0.983194

COD minimum //BP86/AE1

26	0.561283	0.031842	0.023556
6	-1.046998	-0.653573	1.381988
6	-0.945350	0.378912	-1.472809
6	-0.697605	-1.020975	-1.376767
6	-2.199943	1.073811	-0.933170
6	-1.048501	0.757704	1.327354
6	-2.028980	1.590702	0.515742
6	-1.571816	-2.046502	-0.672369
6	-2.079295	-1.543725	0.690086
1	-0.589253	-1.094394	2.275567
1	-0.595399	1.279569	2.180477
1	-1.650300	2.627661	0.487091
1	-3.007243	1.636339	1.041131
1	-3.060519	0.382627	-1.002102
1	-2.448058	1.924067	-1.593225
1	-0.475365	0.882685	-2.326662
1	-0.117839	-1.456933	-2.202929
1	-2.414790	-2.352963	-1.331344
1	-0.962047	-2.954431	-0.514650
1	-2.308973	-2.402229	1.346615
1	-3.027349	-0.986907	0.577028
6	1.800548	-0.432363	-1.151529
6	1.558687	-0.774000	1.259869
6	1.009325	1.764628	0.105967
8	2.629962	-0.724660	-1.926117
8	2.234647	-1.275601	2.077689
8	1.330809	2.890173	0.148976

COD IRC 0.48 //BP86/AE1

26	0.561003	0.039464	-0.001709
6	-0.952535	-0.581949	1.461078
6	-1.033068	0.269356	-1.457537
6	-0.762898	-1.114914	-1.284158
6	-2.263552	0.985083	-0.892782
6	-0.978607	0.827325	1.311373
6	-2.019266	1.594094	0.509173
6	-1.580454	-2.103083	-0.468343
6	-2.013445	-1.523843	0.888326
1	-0.453323	-0.957767	2.362427
1	-0.493653	1.412602	2.104090
1	-1.659935	2.631997	0.392561
1	-2.968767	1.661547	1.082880
1	-3.114972	0.279961	-0.868989
1	-2.559979	1.787143	-1.592014
1	-0.608668	0.720966	-2.362513
1	-0.218417	-1.593357	-2.110396
1	-2.453867	-2.455936	-1.061193
1	-0.950152	-2.993637	-0.294092
1	-2.192236	-2.344518	1.606177
1	-2.975090	-0.985636	0.799686
6	1.737945	-0.743266	-1.072450
6	1.657869	-0.394015	1.325925
6	0.969002	1.762598	-0.283785
8	2.540471	-1.235428	-1.772583
8	2.387374	-0.653730	2.206872
8	1.259283	2.882441	-0.463675

COD IRC 0.40 //BP86/AE1

26	0.560988	0.039420	-0.010215
6	-0.925158	-0.549848	1.485109
6	-1.061411	0.242328	-1.450415
6	-0.789998	-1.136886	-1.253878
6	-2.279955	0.970295	-0.876505
6	-0.952922	0.857212	1.304696
6	-2.005814	1.610261	0.505542
6	-1.593001	-2.107121	-0.403047
6	-1.997327	-1.502618	0.951558
1	-0.413309	-0.906468	2.387290
1	-0.456196	1.459221	2.077543
1	-1.643346	2.643082	0.357014
1	-2.944292	1.696957	1.094748
1	-3.129185	0.264641	-0.818110
1	-2.592155	1.755553	-1.587839
1	-0.650568	0.675611	-2.370366
1	-0.257494	-1.631211	-2.078406
1	-2.478446	-2.468120	-0.972640
1	-0.961192	-2.995953	-0.225801
1	-2.160440	-2.310731	1.687165
1	-2.961473	-0.967015	0.873886
6	1.711069	-0.846501	-1.030519
6	1.683716	-0.281366	1.325704
6	0.970407	1.740243	-0.404099
8	2.500247	-1.404125	-1.696567
8	2.426880	-0.469926	2.212883
8	1.260968	2.846991	-0.651786

COD IRC 0.24 //BP86/AE1

26	0.560873	0.034105	-0.025024
6	-0.880807	-0.494996	1.521261
6	-1.112879	0.224509	-1.431259
6	-0.853778	-1.149704	-1.210298
6	-2.299140	0.983493	-0.832452
6	-0.896323	0.908948	1.300934
6	-1.960997	1.660331	0.516286
6	-1.638209	-2.086878	-0.307029
6	-1.982337	-1.447589	1.048914
1	-0.347271	-0.833310	2.418146
1	-0.373197	1.525556	2.044762
1	-1.579973	2.678527	0.319827
1	-2.876559	1.789666	1.133491
1	-3.151212	0.288501	-0.717574
1	-2.631856	1.749351	-1.555563
1	-0.723899	0.630378	-2.372802
1	-0.346692	-1.668143	-2.035724
1	-2.549144	-2.445198	-0.836499
1	-1.013707	-2.981705	-0.134685
1	-2.125315	-2.239234	1.806270
1	-2.944205	-0.904478	0.997513
6	1.642040	-1.047632	-0.929846
6	1.728284	-0.091479	1.301650
6	1.000397	1.668165	-0.617596
8	2.393352	-1.730928	-1.519259
8	2.495359	-0.158480	2.185013
8	1.311643	2.734451	-0.988246

COD IRC 0.32 //BP86/AE1

26	0.560995	0.037549	-0.018259
6	-0.900880	-0.519673	1.505597
6	-1.088384	0.225935	-1.441575
6	-0.820479	-1.149647	-1.228108
6	-2.292119	0.968797	-0.856639
6	-0.925312	0.885325	1.300459
6	-1.986369	1.632588	0.506851
6	-1.612078	-2.102091	-0.347183
6	-1.986581	-1.476409	1.006647
1	-0.377284	-0.862983	2.406316
1	-0.415735	1.498429	2.056252
1	-1.616646	2.658557	0.330699
1	-2.913441	1.740611	1.110603
1	-3.141460	0.266661	-0.767036
1	-2.616664	1.741277	-1.576397
1	-0.689631	0.643084	-2.374126
1	-0.300510	-1.657955	-2.051974
1	-2.510043	-2.465562	-0.895104
1	-0.981959	-2.992063	-0.169930
1	-2.137494	-2.274140	1.756047
1	-2.950874	-0.939278	0.941219
6	1.679476	-0.948587	-0.982392
6	1.707326	-0.179219	1.316678
6	0.980212	1.708383	-0.516224
8	2.451857	-1.570199	-1.611030
8	2.463016	-0.302680	2.204249
8	1.277250	2.797214	-0.827781

COD IRC 0.16 //BP86/AE1

26	0.560844	0.029027	-0.030980
6	-0.864027	-0.474163	1.533231
6	-1.134625	0.235378	-1.420163
6	-0.889487	-1.139494	-1.198909
6	-2.301002	1.011700	-0.805612
6	-0.865518	0.929535	1.304900
6	-1.929774	1.692918	0.531506
6	-1.671022	-2.062872	-0.279188
6	-1.983733	-1.415771	1.081231
1	-0.322001	-0.814262	2.424433
1	-0.328187	1.543710	2.040813
1	-1.534001	2.702567	0.320298
1	-2.833527	1.843591	1.161386
1	-3.158175	0.326846	-0.670289
1	-2.638008	1.776050	-1.528351
1	-0.753292	0.633658	-2.368002
1	-0.395743	-1.665429	-2.027526
1	-2.595493	-2.409236	-0.792754
1	-1.056442	-2.966092	-0.115469
1	-2.122766	-2.204633	1.842199
1	-2.940658	-0.862676	1.045086
6	1.598048	-1.144404	-0.873544
6	1.748362	-0.016087	1.281506
6	1.028835	1.620757	-0.709462
8	2.323227	-1.887763	-1.421923
8	2.526896	-0.033354	2.156697
8	1.359877	2.660645	-1.134689

COD IRC 0.08 //BP86/AE1

26	0.560747	0.022851	-0.035342
6	-0.852059	-0.459306	1.540564
6	-1.152006	0.261158	-1.408639
6	-0.926051	-1.116650	-1.196237
6	-2.296764	1.054468	-0.776120
6	-0.834191	0.945305	1.313701
6	-1.893314	1.729339	0.554143
6	-1.709586	-2.029516	-0.267866
6	-1.991600	-1.382756	1.100126
1	-0.304243	-0.809329	2.424429
1	-0.282709	1.550008	2.047210
1	-1.479356	2.730152	0.335604
1	-2.785447	1.899918	1.195661
1	-3.161417	0.382103	-0.626954
1	-2.633593	1.823454	-1.494040
1	-0.775364	0.657263	-2.359228
1	-0.445446	-1.645987	-2.030262
1	-2.647314	-2.357058	-0.769388
1	-1.108910	-2.944199	-0.117016
1	-2.131313	-2.173345	1.859156
1	-2.941118	-0.816152	1.080392
6	1.546798	-1.237298	-0.814711
6	1.766515	0.044919	1.259774
6	1.067041	1.566638	-0.790974
8	2.240317	-2.038252	-1.321519
8	2.556010	0.068888	2.124484
8	1.424687	2.575768	-1.266620

COD minimum //BP86/ECP2

26	0.562594	0.030175	0.024152
6	-1.050154	-0.654372	1.384606
6	-0.947060	0.387897	-1.470245
6	-0.708177	-1.008792	-1.381976
6	-2.193494	1.086501	-0.924524
6	-1.048039	0.751908	1.335857
6	-2.028208	1.584928	0.529731
6	-1.584508	-2.029406	-0.679421
6	-2.082613	-1.535329	0.687159
1	-0.589939	-1.101211	2.271400
1	-0.583823	1.269762	2.182941
1	-1.664816	2.625313	0.518489
1	-3.006745	1.616246	1.051727
1	-3.058283	0.405586	-1.006738
1	-2.433569	1.943346	-1.575301
1	-0.469885	0.894073	-2.316188
1	-0.128602	-1.442797	-2.206539
1	-2.430746	-2.322939	-1.337025
1	-0.986363	-2.944655	-0.535439
1	-2.314387	-2.396244	1.336218
1	-3.028568	-0.977384	0.583402
6	1.794309	-0.444523	-1.140567
6	1.559419	-0.769494	1.253544
6	1.016971	1.755052	0.094175
8	2.619730	-0.741400	-1.905389
8	2.237231	-1.263637	2.062734
8	1.355241	2.867552	0.127038

COD TS //BP86/AE1

26	0.560608	0.015658	-0.038515
6	-0.845339	-0.448744	1.543723
6	-1.164510	0.299611	-1.397227
6	-0.962348	-1.082755	-1.201046
6	-2.286308	1.109459	-0.745481
6	-0.802858	0.957393	1.325944
6	-1.851726	1.769321	0.581699
6	-1.752635	-1.987681	-0.270705
6	-2.005713	-1.347998	1.107084
1	-0.295005	-0.815371	2.419314
1	-0.237658	1.546456	2.061940
1	-1.416028	2.760566	0.361632
1	-2.732379	1.959215	1.233828
1	-3.160531	0.451666	-0.587818
1	-2.618781	1.887867	-1.455276
1	-0.789398	0.698051	-2.347421
1	-0.494330	-1.612135	-2.042053
1	-2.702792	-2.291016	-0.763707
1	-1.169218	-2.915839	-0.135568
1	-2.150682	-2.143735	1.859699
1	-2.945597	-0.765202	1.103991
6	1.488247	-1.326527	-0.753205
6	1.782741	0.093416	1.237985
6	1.114233	1.505684	-0.863640
8	2.144401	-2.182806	-1.217425
8	2.582638	0.151555	2.091068
8	1.504697	2.479413	-1.385888

COD IRC 0.68 //BP86/ECP2

26	0.562469	0.031755	0.019491
6	-1.031787	-0.645926	1.398817
6	-0.962928	0.366857	-1.467684
6	-0.719113	-1.027582	-1.366263
6	-2.205836	1.067793	-0.917148
6	-1.035245	0.760758	1.334310
6	-2.029262	1.580235	0.531135
6	-1.584108	-2.043830	-0.643829
6	-2.069745	-1.536867	0.722142
1	-0.563368	-1.081965	2.286734
1	-0.564996	1.290316	2.170812
1	-1.673059	2.622899	0.506955
1	-3.003081	1.609742	1.061946
1	-3.069399	0.383812	-0.985480
1	-2.453621	1.917709	-1.574068
1	-0.494561	0.864583	-2.323446
1	-0.146604	-1.468024	-2.192288
1	-2.435284	-2.347556	-1.290377
1	-0.980720	-2.955051	-0.496322
1	-2.292754	-2.391502	1.382475
1	-3.018244	-0.982447	0.622217
6	1.783781	-0.502783	-1.131274
6	1.581322	-0.694618	1.274366
6	1.004664	1.761554	0.019715
8	2.605281	-0.836724	-1.885372
8	2.271104	-1.140550	2.101083
8	1.333748	2.877060	0.009085

COD IRC 0.56 //BP86/ECP2

26	0.562435	0.034891	0.006596
6	-0.985483	-0.605055	1.439653
6	-1.005143	0.306035	-1.462954
6	-0.751766	-1.080840	-1.317031
6	-2.235398	1.021745	-0.904128
6	-0.999911	0.800756	1.322714
6	-2.023483	1.584435	0.520744
6	-1.589589	-2.075176	-0.535264
6	-2.039075	-1.523285	0.824970
1	-0.496775	-1.006415	2.333100
1	-0.514008	1.364871	2.127252
1	-1.676669	2.628268	0.450555
1	-2.983443	1.625422	1.075523
1	-3.096831	0.332184	-0.926329
1	-2.503682	1.846941	-1.584070
1	-0.558429	0.773830	-2.346561
1	-0.196959	-1.546178	-2.141288
1	-2.455666	-2.404928	-1.148481
1	-0.976755	-2.977656	-0.374029
1	-2.239544	-2.355732	1.519953
1	-2.992973	-0.976539	0.732987
6	1.753413	-0.658374	-1.093169
6	1.630150	-0.504426	1.310035
6	0.984135	1.761014	-0.173675
8	2.562459	-1.091218	-1.810624
8	2.345685	-0.829719	2.169918
8	1.297023	2.874411	-0.294477

COD IRC 0.32 //BP86/ECP2

26	0.562987	0.033376	-0.019262
6	-0.903413	-0.503815	1.511287
6	-1.088910	0.220332	-1.444037
6	-0.833940	-1.151176	-1.223841
6	-2.282052	0.977471	-0.862696
6	-0.921335	0.894874	1.297947
6	-1.981160	1.635820	0.502658
6	-1.628764	-2.087865	-0.334327
6	-1.992348	-1.454648	1.016428
1	-0.376826	-0.846024	2.408176
1	-0.400728	1.510641	2.041086
1	-1.624024	2.665353	0.335676
1	-2.908272	1.734935	1.104432
1	-3.140110	0.288373	-0.781880
1	-2.593623	1.752282	-1.582299
1	-0.681946	0.629362	-2.374448
1	-0.315145	-1.667106	-2.040949
1	-2.530948	-2.443229	-0.876997
1	-1.012985	-2.985519	-0.158860
1	-2.148468	-2.246270	1.768131
1	-2.952104	-0.913562	0.953427
6	1.671315	-0.967988	-0.964078
6	1.708687	-0.166522	1.306885
6	0.988192	1.691371	-0.529988
8	2.439478	-1.594964	-1.577496
8	2.464768	-0.279079	2.184632
8	1.299491	2.764775	-0.851150

COD IRC 0.44 //BP86/ECP2

26	0.562593	0.035411	-0.006628
6	-0.941999	-0.552472	1.479552
6	-1.047841	0.252383	-1.455497
6	-0.790274	-1.125930	-1.265675
6	-2.261628	0.988024	-0.887965
6	-0.961732	0.849991	1.308144
6	-2.007253	1.604831	0.506799
6	-1.604216	-2.090918	-0.424712
6	-2.012222	-1.493033	0.929055
1	-0.433671	-0.919124	2.377127
1	-0.458997	1.445529	2.079250
1	-1.659293	2.643631	0.384678
1	-2.951347	1.672183	1.085874
1	-3.120633	0.295945	-0.856728
1	-2.552687	1.785131	-1.591616
1	-0.622031	0.687764	-2.365435
1	-0.253546	-1.619065	-2.085501
1	-2.487770	-2.439504	-1.001484
1	-0.987068	-2.988294	-0.252252
1	-2.189016	-2.302407	1.656923
1	-2.970507	-0.951857	0.848860
6	1.716274	-0.817366	-1.035076
6	1.672157	-0.322966	1.320167
6	0.978460	1.735691	-0.362619
8	2.507975	-1.350085	-1.704106
8	2.409346	-0.533850	2.196595
8	1.285278	2.833929	-0.590040

COD IRC 0.20 //BP86/ECP2

26	0.563366	0.028133	-0.029818
6	-0.872683	-0.468679	1.532634
6	-1.125556	0.220060	-1.429020
6	-0.883260	-1.149309	-1.199412
6	-2.292473	0.999938	-0.826347
6	-0.877854	0.928391	1.298483
6	-1.942660	1.676759	0.517177
6	-1.666873	-2.064111	-0.278043
6	-1.984625	-1.412846	1.076425
1	-0.330841	-0.804316	2.423085
1	-0.337844	1.548029	2.024677
1	-1.567524	2.694685	0.320448
1	-2.852220	1.808044	1.139544
1	-3.154183	0.321096	-0.707819
1	-2.617036	1.765371	-1.550264
1	-0.733385	0.613747	-2.372202
1	-0.382826	-1.679009	-2.018947
1	-2.588397	-2.410312	-0.793229
1	-1.060340	-2.969531	-0.110882
1	-2.128165	-2.196355	1.839026
1	-2.940706	-0.863044	1.035309
6	1.614797	-1.109767	-0.885396
6	1.740644	-0.041811	1.279020
6	1.017112	1.631533	-0.672193
8	2.350644	-1.824809	-1.439992
8	2.513770	-0.074834	2.147729
8	1.346401	2.672043	-1.074419

COD IRC 0.08 //BP86/ECP2

26	0.563702	0.020133	-0.037905
6	-0.850473	-0.447962	1.544374
6	-1.155175	0.251971	-1.412045
6	-0.936313	-1.120417	-1.193577
6	-2.291023	1.054270	-0.781334
6	-0.831665	0.950253	1.310443
6	-1.891927	1.725852	0.549937
6	-1.717980	-2.020857	-0.256798
6	-1.989660	-1.369544	1.108653
1	-0.297673	-0.795097	2.423767
1	-0.271497	1.558185	2.031542
1	-1.490983	2.731159	0.339233
1	-2.783681	1.887038	1.191112
1	-3.161257	0.391371	-0.638316
1	-2.619946	1.823882	-1.498881
1	-0.772797	0.642063	-2.360650
1	-0.454466	-1.654841	-2.020965
1	-2.658976	-2.342632	-0.751903
1	-1.129221	-2.941090	-0.108524
1	-2.129735	-2.155110	1.869748
1	-2.936731	-0.802980	1.093283
6	1.543838	-1.243150	-0.802609
6	1.769639	0.051305	1.243857
6	1.064791	1.559299	-0.790700
8	2.236415	-2.040915	-1.297176
8	2.559399	0.079609	2.096957
8	1.424986	2.559865	-1.262922

COD TS //BP86/ECP2

26	0.563802	0.013624	-0.041849
6	-0.841863	-0.441272	1.546791
6	-1.169571	0.290213	-1.400435
6	-0.971683	-1.086492	-1.199936
6	-2.283028	1.105986	-0.748212
6	-0.800878	0.958880	1.323866
6	-1.852025	1.762344	0.579865
6	-1.757653	-1.981735	-0.261906
6	-2.000424	-1.340253	1.114452
1	-0.285496	-0.805083	2.417236
1	-0.227728	1.550789	2.048270
1	-1.429475	2.758490	0.367626
1	-2.731967	1.942366	1.232493
1	-3.161125	0.455835	-0.595630
1	-2.610378	1.884867	-1.456476
1	-0.790077	0.684576	-2.348392
1	-0.501469	-1.619061	-2.035073
1	-2.710763	-2.280153	-0.748084
1	-1.184817	-2.914504	-0.130981
1	-2.143311	-2.132435	1.868107
1	-2.938955	-0.759460	1.117576
6	1.488418	-1.326794	-0.745925
6	1.786294	0.096480	1.220586
6	1.107472	1.504491	-0.857906
8	2.145950	-2.176443	-1.200175
8	2.586287	0.155993	2.062111
8	1.496057	2.474008	-1.371442