Table S1. The geometries of optimized and C_s Fischer-Type Chromium-Carbene Complexes $(CO)_5Cr=C(X)R$. Labels according to Table 1.

COMPLEX A

opt

Cr	0.0124	0.0317	0.1801
C	-0.2009	-0.0772	2.0743
C	1.9057	0.0768	0.3552
C	-1.8719	0.0103	-0.0647
O	3.0599	0.1123	0.4272
O	-0.3270	-0.1225	3.2242
O	-3.0180	-0.0078	-0.2305
C	-0.0047	1.9272	0.2511
C	0.0270	-1.8545	0.0427
O	-0.0245	3.0835	0.2980
O	0.0333	-3.0099	-0.0539
C	0.2184	0.1185	-1.7723
O	0.7191	1.1407	-2.4396
C	0.8067	1.0394	-3.8972
H	1.2469	1.9822	-4.2338
H	1.4537	0.1954	-4.1620
H	-0.2006	0.9146	-4.3107
H	-0.0753	-0.6982	-2.4663

Cs

Cr	0.000000	0.000000	0.000000
C	1.901900	0.000000	0.000000
C	0.000000	1.909300	0.000000
O	3.058900	0.000000	0.000000
O	0.000000	3.067000	0.000000
C	-0.000000	0.000000	1.896900
O	-0.000000	0.000000	3.054300
C	-1.901900	0.000000	0.000000
O	-3.058900	0.000000	0.000000
C	-0.000000	0.000000	-1.891300
O	-0.000000	0.000000	-3.050700
C	0.000000	-1.965200	-0.000000
H	0.000000	-2.520850	-0.962414
O	0.000000	-2.624900	1.142634
C	0.000000	-4.088600	1.142634
H	0.820200	-4.635400	1.616177
H	-0.820200	-4.635400	1.616177
H	0.000000	-4.635400	0.195549

COMPLEX B

opt

C	-0.3242	-0.2067	0.3862
Cr	-0.3376	-0.1178	2.2839
C	-0.4045	-0.0123	4.1750
C	1.3456	-1.0258	2.3766
C	-2.0683	0.7768	2.2376
C	-1.2652	-1.7710	2.3865
C	0.5352	1.5684	2.1665
O	-0.3176	-0.2592	-0.7691
O	2.3642	-1.5718	2.4278
O	-1.8435	-2.7716	2.4622
O	1.0513	2.6006	2.0924

O	-0.4733	0.0416	5.3302
O	-2.4573	1.6809	1.3329
H	-3.3788	1.9931	1.5150
H	-2.8777	0.5953	2.9719
Cs			
Cr	0.000000	0.000000	0.000000
C	1.898400	0.000000	0.000000
C	0.000000	1.914700	0.000000
O	3.056600	0.000000	0.000000
O	0.000000	3.071500	0.000000
C	-0.000000	0.000000	1.899800
O	-0.000000	0.000000	3.056300
C	-1.898400	0.000000	0.000000
O	-3.056600	0.000000	0.000000
C	-0.000000	0.000000	-1.895200
O	-0.000000	0.000000	-3.053700
C	0.000000	-1.948800	-0.000000
H	0.000000	-2.502700	-0.959383
O	0.000000	-2.617250	1.157789
H	0.000000	-3.607050	1.157789

COMPLEX C

opt

Cr	0.0400	0.0268	0.2125
C	-0.2244	-0.0943	2.0817
C	1.9242	0.0342	0.4279
C	-1.8283	0.0543	-0.1120
O	3.0784	0.0504	0.5357
O	-0.3870	-0.1544	3.2290
O	-2.9657	0.0832	-0.3340
C	0.0313	1.9033	0.2914
C	0.0434	-1.8628	0.0798
O	0.0265	3.0685	0.3003
O	0.0435	-3.0192	-0.0061
C	0.3504	0.1052	-1.7908
N	0.4037	1.1565	-2.5811
H	0.2603	2.0791	-2.1550
C	0.6344	1.1686	-4.0252
H	1.4680	1.8433	-4.2630
H	0.8856	0.1531	-4.3528
H	-0.2691	1.5097	-4.5501
H	0.5193	-0.8082	-2.3874
Cs			
Cr	0.000000	0.000000	0.000000
C	1.896500	0.000000	0.000000
C	0.000000	1.891700	0.000000
O	3.055800	0.000000	0.000000
O	0.000000	3.052000	0.000000
C	-0.000000	0.000000	1.878200
O	-0.000000	0.000000	3.043400
C	-1.896500	0.000000	0.000000
O	-3.055800	0.000000	0.000000
C	-0.000000	0.000000	-1.894300
O	-0.000000	0.000000	-3.053900
C	0.000000	-2.028700	-0.000000
H	0.000000	-2.580700	-0.956092

N	0.000000	-2.686850	1.139949
C	0.000000	-4.149350	1.139949
H	0.823875	-4.698600	1.615614
H	-0.823875	-4.698600	1.615614
H	0.000000	-4.698600	0.188620
H	0.000000	-2.173700	2.028751

COMPLEX D

opt

C	-0.5441	-0.2028	0.4958
Cr	-0.3099	-0.1686	2.3773
C	-0.1325	-0.1013	4.2529
C	1.3982	-0.9712	2.1817
C	-2.1181	0.6913	2.4998
C	-1.1423	-1.8578	2.5566
C	0.4297	1.5747	2.2452
O	-0.6893	-0.2127	-0.6539
O	2.4338	-1.4766	2.0580
O	-1.6931	-2.8690	2.6980
O	0.8629	2.6465	2.1668
O	-0.0666	-0.0606	5.4125
H	-2.4917	1.3665	1.7110
N	-3.0425	0.5840	3.4482
H	-3.9413	1.0666	3.4045
H	-2.8830	0.0066	4.2733

Cs

Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.891700
C	1.897400	0.000000	0.000000
O	0.000000	0.000000	3.051800
O	3.056400	0.000000	0.000000
C	0.000000	1.885200	0.000000
O	0.000000	3.047400	0.000000
C	0.000000	0.000000	-1.891700
O	0.000000	0.000000	-3.051800
C	0.000000	-1.896300	0.000000
O	0.000000	-3.055200	0.000000
C	-2.006000	-0.000000	0.000000
H	-2.557750	-0.955659	0.000000
N	-2.670350	1.150688	0.000000
H	-3.689950	1.150688	0.000000
H	-2.159800	2.034986	0.000000

COMPLEX E

opt

C	-0.3241	-0.1688	0.3902
Cr	-0.3316	-0.1096	2.2948
C	-0.4065	-0.0405	4.1973
C	1.3660	-1.0390	2.3616
C	-2.0073	0.8132	2.2210
C	-1.2773	-1.7576	2.4288
C	0.5535	1.5737	2.1750
O	-0.3335	-0.1837	-0.7651
O	2.3779	-1.5930	2.3993
O	-1.8626	-2.7484	2.5345
O	1.0682	2.6045	2.0884

O	-0.4870	-0.0215	5.3498
H	-2.2414	1.6410	1.5306
H	-2.8782	0.5938	2.8614
Cs			
Cr	0.000000	0.000000	0.000000
C	1.905500	0.000000	0.000000
C	0.000000	1.936516	0.000000
O	3.060934	0.000000	0.000000
O	0.000000	3.090716	0.000000
C	-0.000000	0.000000	1.905500
O	-0.000000	0.000000	3.061000
C	-1.905600	0.000000	0.000000
O	-3.061000	0.000000	0.000000
C	-0.000000	0.000000	-1.904800
O	-0.000000	0.000000	-3.060400
C	0.000000	-1.914400	0.000000
H	0.000000	-2.465900	-0.955226
H	0.000000	-2.465900	0.955226

COMPLEX F

opt

Cr	-0.0057	0.0058	0.1679
C	-0.1830	-0.0412	2.0582
C	1.8876	0.0416	0.2693
C	-1.8852	-0.0166	-0.0855
O	3.0462	0.0688	0.2828
O	-0.2832	-0.0704	3.2128
O	-3.0304	-0.0394	-0.2670
C	-0.0185	1.9027	0.2156
C	0.0109	-1.8814	0.1558
O	-0.0263	3.0597	0.2662
O	0.0114	-3.0433	0.1619
C	0.2064	0.0591	-1.8302
O	0.6906	1.1687	-2.3774
C	0.9418	1.3056	-3.8107
H	1.3963	2.2951	-3.9137
H	1.6342	0.5292	-4.1549
H	-0.0026	1.2663	-4.3655
C	-0.0710	-1.0727	-2.7698
H	-0.8044	-1.7624	-2.3388
H	-0.4066	-0.7643	-3.7714
H	0.8704	-1.6420	-2.8929
Cs			
Cr	0.000000	0.000000	0.000000
C	1.896400	0.000000	0.000000
C	0.000000	1.899200	0.000000
O	3.055400	0.000000	0.000000
O	0.000000	3.058500	0.000000
C	0.000000	0.000000	1.897500
O	0.000000	0.000000	3.055600
C	-1.896400	0.000000	0.000000
O	-3.055400	0.000000	0.000000
C	0.000000	0.000000	-1.887300
O	0.000000	0.000000	-3.049200
C	0.000000	-2.010000	-0.000000
C	0.000000	-2.758450	-1.296353

O	0.000000	-2.679300	1.159262
C	0.000000	-4.140900	1.159262
H	0.820350	-4.687800	1.632891
H	-0.820350	-4.687800	1.632891
H	0.000000	-4.687800	0.212003
H	-0.825300	-2.620900	-2.011084
H	0.825300	-2.620900	-2.011084
H	0.000000	-3.858850	-1.296353

COMPLEX G

opt

Cr	0.0003	0.0090	0.1663
C	-0.1869	-0.0385	2.0603
C	1.8960	0.0484	0.2829
C	-1.8818	-0.0228	-0.0774
O	3.0531	0.0748	0.3100
O	-0.2988	-0.0675	3.2128
O	-3.0262	-0.0546	-0.2575
C	-0.0156	1.9074	0.2126
C	0.0178	-1.8797	0.1432
O	-0.0246	3.0637	0.2610
O	0.0203	-3.0409	0.1406
C	0.1989	0.0577	-1.8132
O	0.7114	1.1376	-2.4142
H	0.7486	1.0141	-3.3997
C	-0.1137	-1.0412	-2.7802
H	-0.9138	-1.6976	-2.4197
H	-0.3782	-0.6614	-3.7848
H	0.7964	-1.6621	-2.8782

Cs

Cr	0.000000	0.000000	0.000000
C	1.899700	0.000000	0.000000
C	0.000000	1.903800	0.000000
O	3.057400	0.000000	0.000000
O	0.000000	3.062100	0.000000
C	0.000000	0.000000	1.899000
O	0.000000	0.000000	3.056300
C	-1.899700	0.000000	0.000000
O	-3.057400	0.000000	0.000000
C	0.000000	0.000000	-1.888900
O	0.000000	0.000000	-3.050100
C	0.000000	-1.990000	-0.000000
C	0.000000	-2.738400	-1.296267
O	0.000000	-2.658950	1.158655
H	0.000000	-3.652850	1.158655
H	-0.829575	-2.600138	-2.014700
H	0.829575	-2.600138	-2.014700
H	0.000000	-3.844500	-1.296267

COMPLEX H

opt

Cr	-0.0047	0.0171	0.1936
C	-0.1650	-0.0562	2.0707
C	1.8842	0.0232	0.2599
C	-1.8769	0.0010	-0.0902
O	3.0451	0.0296	0.2424

O	-0.2501	-0.0905	3.2283
O	-3.0191	-0.0238	-0.2934
C	-0.0498	1.8938	0.2920
C	-0.0178	-1.8750	0.1786
O	-0.0833	3.0576	0.3391
O	-0.0522	-3.0355	0.2048
C	0.2399	0.0798	-1.8664
N	0.6426	1.1720	-2.4959
H	0.7868	2.0020	-1.9174
C	0.9478	1.3569	-3.9223
H	1.3455	2.3697	-4.0525
H	1.7068	0.6371	-4.2545
H	0.0432	1.2535	-4.5361
C	0.0508	-1.1240	-2.7398
H	-0.8379	-1.6842	-2.4228
H	-0.0224	-0.9194	-3.8181
H	0.9106	-1.7970	-2.5766

Cs

Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.893700
C	1.885400	0.000000	0.000000
O	0.000000	0.000000	3.054100
O	3.046600	0.000000	0.000000
C	0.000000	1.879800	0.000000
O	0.000000	3.045000	0.000000
C	0.000000	0.000000	-1.893700
O	0.000000	0.000000	-3.054100
C	0.000000	-1.892200	0.000000
O	0.000000	-3.053500	0.000000
C	-2.075400	-0.000000	0.000000
C	-2.825000	-1.298345	0.000000
N	-2.737100	1.146098	0.000000
C	-4.207500	1.146098	0.000000
H	-4.755400	0.671603	0.821850
H	-4.755400	2.095089	0.000000
H	-4.755400	0.671603	-0.821850
H	-2.226150	2.031089	0.000000
H	-2.687838	-2.011063	-0.822975
H	-2.687838	-2.011063	0.822975
H	-3.922300	-1.298345	0.000000

COMPLEX I

opt

Cr	-0.0001	0.0164	0.1915
C	-0.1734	-0.0502	2.0706
C	1.8896	0.0248	0.2723
C	-1.8742	0.0009	-0.0913
O	3.0499	0.0338	0.2628
O	-0.2687	-0.0824	3.2266
O	-3.0163	-0.0222	-0.2917
C	-0.0399	1.8950	0.2853
C	-0.0101	-1.8756	0.1696
O	-0.0650	3.0576	0.3416
O	-0.0344	-3.0362	0.1812
C	0.2317	0.0764	-1.8476
N	0.6156	1.1526	-2.5148

H	0.8140	2.0308	-2.0340
H	0.7478	1.1480	-3.5327
C	0.0378	-1.1120	-2.7414
H	-0.8730	-1.6603	-2.4695
H	0.0012	-0.8614	-3.8168
H	0.8803	-1.8036	-2.5744
Cs			
Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.895400
C	1.888200	0.000000	0.000000
O	0.000000	0.000000	3.055200
O	3.048600	0.000000	0.000000
C	0.000000	1.881400	0.000000
O	0.000000	3.045600	0.000000
C	0.000000	0.000000	-1.895400
O	0.000000	0.000000	-3.055200
C	0.000000	-1.892200	0.000000
O	0.000000	-3.053100	0.000000
C	-2.053100	-0.000000	0.000000
C	-2.802900	-1.298692	0.000000
N	-2.714700	1.145925	0.000000
H	-3.741200	1.145925	0.000000
H	-2.204350	2.029877	0.000000
H	-2.664800	-2.016280	-0.828600
H	-2.664800	-2.016280	0.828600
H	-3.907700	-1.298692	0.000000

COMPLEX J

opt

Cr	0.0168	-0.0099	0.1952
C	-0.1849	-0.0328	2.1113
C	1.9094	0.0563	0.3769
C	-1.8632	-0.0630	-0.0846
O	3.0618	0.1154	0.4579
O	-0.2833	-0.0674	3.2624
O	-2.9999	-0.1177	-0.2927
C	0.0133	1.8916	0.1638
C	0.0016	-1.9055	0.1499
O	0.0266	3.0478	0.1247
O	-0.0289	-3.0615	0.0933
C	0.2850	0.0021	-1.7267
H	0.9691	0.7440	-2.1800
C	-0.2584	-0.8807	-2.7817
H	-1.0095	-1.6038	-2.4405
H	-0.6657	-0.2804	-3.6175
H	0.5918	-1.4363	-3.2293
Cs			
Cr	0.000000	0.000000	0.000000
C	1.901400	0.000000	0.000000
C	0.000000	1.926800	0.000000
O	3.058300	0.000000	0.000000
O	0.000000	3.082600	0.000000
C	0.000000	0.000000	1.896200
O	0.000000	0.000000	3.054000
C	-1.901400	0.000000	0.000000
O	-3.058300	0.000000	0.000000

C	0.000000	0.000000	-1.901800
O	0.000000	0.000000	-3.058700
C	0.000000	-1.940600	-0.000000
C	0.000000	-2.680150	-1.280938
H	0.000000	-2.493750	0.958084
H	-0.822750	-2.543025	-1.993461
H	0.822750	-2.543025	-1.993461
H	0.000000	-3.777150	-1.280938

COMPLEX K

opt

Cr	0.0222	-0.0224	0.1836
C	-0.2102	-0.0155	2.0701
C	1.9136	0.0819	0.3158
C	-1.8460	-0.1040	-0.1227
O	3.0695	0.1541	0.3362
O	-0.3466	-0.0123	3.2209
O	-2.9829	-0.1635	-0.3444
C	-0.0482	1.8731	0.1728
C	0.0917	-1.9160	0.2442
O	-0.0941	3.0301	0.1836
O	0.1240	-3.0734	0.3128
C	0.2784	-0.0172	-1.8072
O	0.7252	1.0761	-2.4097
C	0.8424	1.2252	-3.8620
H	0.5439	2.2601	-4.0590
H	1.8918	1.0774	-4.1388
H	0.1964	0.5158	-4.3869
C	0.0502	-1.2293	-2.6049
H	-0.9175	-1.7136	-2.4394
H	0.8071	-2.8463	-3.7472
C	0.9944	-1.8615	-3.3179
H	2.0000	-1.4520	-3.4327

Cs

Cr	0.000000	0.000000	0.000000
C	1.898900	0.000000	0.000000
C	0.000000	1.900800	0.000000
O	3.057200	0.000000	0.000000
O	0.000000	3.059700	0.000000
C	0.000000	0.000000	1.896800
O	0.000000	0.000000	3.054800
C	-1.898900	0.000000	0.000000
O	-3.057200	0.000000	0.000000
C	0.000000	0.000000	-1.895800
O	0.000000	0.000000	-3.055700
C	0.000000	-2.007200	-0.000000
C	0.000000	-2.741650	-1.272105
O	0.000000	-2.670150	1.148263
C	0.000000	-4.129177	1.275911
H	0.821250	-4.715918	0.851285
H	0.000000	-4.591944	2.268318
H	-0.821250	-4.715918	0.851285
H	0.000000	-2.194300	-2.220143
C	0.000000	-4.083150	-1.272105
H	0.000000	-4.629050	-0.326578
H	0.000000	-4.629050	-2.217631

COMPLEX L

opt

C	-0.443900	-0.226200	0.451400
Cr	-0.338000	-0.120100	2.347600
C	-0.228600	0.013700	4.230800
C	1.335700	-1.022300	2.313300
C	-2.100100	0.847700	2.326700
C	-1.243200	-1.771900	2.515700
C	0.525100	1.565400	2.170800
O	-0.504500	-0.289700	-0.701900
O	2.353400	-1.575200	2.292500
O	-1.802200	-2.780600	2.638300
O	1.046900	2.591900	2.063400
O	-0.157600	0.085300	5.386600
O	-2.254200	1.833000	1.420800
H	-3.159100	2.239100	1.482000
C	-3.316700	0.662800	3.118400
H	-3.197263	0.087439	4.052297
H	-5.384729	0.897653	3.487422
C	-4.547708	1.106778	2.820953
H	-4.762778	1.674638	1.918303

Cs

Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.890700
C	1.906400	0.000000	0.000000
O	0.000000	0.000000	3.050700
O	3.064200	0.000000	0.000000
C	0.000000	1.900000	0.000000
O	0.000000	3.056500	0.000000
C	0.000000	0.000000	-1.890700
O	0.000000	0.000000	-3.050700
C	0.000000	-1.901700	0.000000
O	0.000000	-3.059800	0.000000
C	-1.989500	-0.000000	0.000000
C	-2.809389	-1.215535	0.000000
O	-2.660300	1.161860	0.000000
H	-2.330600	-2.197198	0.000000
C	-4.154584	-1.192054	0.000000
H	-4.684675	-0.235745	0.000000
H	-4.716078	-2.126538	0.000000
H	-3.639691	0.989167	0.000000

COMPLEX M

opt

Cr	0.0217	-0.0121	0.2020
C	-0.1917	-0.0343	2.0754
C	1.9086	0.0598	0.3194
C	-1.8429	-0.0868	-0.1165
O	3.0675	0.1182	0.3409
O	-0.3117	-0.0373	3.2301
O	-2.9800	-0.1340	-0.3429
C	-0.0718	1.8639	0.2388
C	0.0766	-1.9117	0.2382
O	-0.1347	3.0272	0.2420
O	0.0949	-3.0688	0.3055

C	0.2864	0.0189	-1.8505
N	0.6762	1.0817	-2.5335
H	0.8529	1.9275	-1.9843
C	0.8533	1.2517	-3.9795
H	0.4081	2.2110	-4.2741
H	1.9214	1.2573	-4.2375
H	0.3568	0.4340	-4.5106
C	0.0845	-1.2252	-2.6029
H	-0.9109	-1.6707	-2.5030
H	0.8738	-2.9014	-3.6309
C	1.0583	-1.9088	-3.2191
H	2.0822	-1.5316	-3.2641

Cs

Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.893100
C	1.885600	0.000000	0.000000
O	0.000000	0.000000	3.053500
O	3.046500	0.000000	0.000000
C	0.000000	1.878700	0.000000
O	0.000000	3.043700	0.000000
C	0.000000	0.000000	-1.893100
O	0.000000	0.000000	-3.053500
C	0.000000	-1.900700	0.000000
O	0.000000	-3.059900	0.000000
C	-2.069700	-0.000000	0.000000
C	-2.803650	-1.271239	0.000000
N	-2.730750	1.144972	0.000000
C	-4.197450	1.144972	0.000000
H	-4.746350	0.669611	0.823350
H	-4.746350	2.095695	0.000000
H	-4.746350	0.669611	-0.823350
H	-2.218850	2.031609	0.000000
C	-4.138451	-1.388019	0.000000
H	-2.256100	-2.219623	0.000000
H	-4.763879	-0.494815	0.000000
H	-4.599274	-2.376257	0.000000

COMPLEX N

opt

Cr	0.0226	-0.0153	0.2123
C	-0.2042	-0.0168	2.0892
C	1.9105	0.0629	0.3459
C	-1.8423	-0.0972	-0.1122
O	3.0683	0.1244	0.3734
O	-0.3335	-0.0072	3.2418
O	-2.9761	-0.1504	-0.3503
C	-0.0662	1.8639	0.2220
C	0.0860	-1.9142	0.2590
O	-0.1233	3.0261	0.2153
O	0.1134	-3.0710	0.3242
C	0.2841	-0.0116	-1.8164
N	0.7228	1.0074	-2.5406
H	0.9625	1.9001	-2.1072
H	0.8033	0.9456	-3.5614
C	0.0616	-1.2295	-2.6042
H	-0.8934	-1.7373	-2.4439

H	0.8362	-2.7572	-3.8558
C	1.0064	-1.7966	-3.3693
H	2.0029	-1.3584	-3.4630
Cs			
Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.894700
C	1.890600	0.000000	0.000000
O	0.000000	0.000000	3.054500
O	3.050500	0.000000	0.000000
C	0.000000	1.881300	0.000000
O	0.000000	3.044900	0.000000
C	0.000000	0.000000	-1.894700
O	0.000000	0.000000	-3.054500
C	0.000000	-1.900500	0.000000
O	0.000000	-3.059500	0.000000
C	-2.045500	-0.000000	0.000000
C	-2.779250	-1.270892	0.000000
N	-2.707950	1.147397	0.000000
H	-3.733750	1.147397	0.000000
H	-2.197500	2.031522	0.000000
C	-4.115645	-1.387812	0.000000
H	-2.232550	-2.217804	0.000000
H	-4.742335	-0.492806	0.000000
H	-4.577398	-2.378044	0.000000

COMPLEX O

opt			
C	-0.447800	-0.209400	0.451200
Cr	-0.324300	-0.125100	2.354000
C	-0.211100	-0.027800	4.245400
C	1.373000	-1.022100	2.286800
C	-2.050000	0.831600	2.354700
C	-1.255700	-1.762400	2.551200
C	0.511700	1.575900	2.177400
O	-0.515000	-0.247100	-0.702000
O	2.389200	-1.572900	2.258700
O	-1.856700	-2.740600	2.698800
O	1.008400	2.614400	2.066300
O	-0.156500	0.025400	5.400600
H	-2.147600	1.666300	1.640400
C	-3.296800	0.666400	3.059100
C	-4.502408	1.465418	2.530253
H	-4.202451	2.043557	1.681323
H	-5.360807	1.257388	3.134219
H	-3.380504	0.020247	3.907852
Cs			
Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.901100
C	1.924300	0.000000	0.000000
O	0.000000	0.000000	3.058100
O	3.080300	0.000000	0.000000
C	0.000000	1.903500	0.000000
O	0.000000	3.060000	0.000000
C	0.000000	0.000000	-1.901100
O	0.000000	0.000000	-3.058100
C	0.000000	-1.899900	0.000000

O	0.000000	-3.057000	0.000000
C	-1.959500	-0.000000	0.000000
C	-2.973845	-1.014345	0.000000
H	-2.511950	0.956871	0.000000
H	-2.690490	-2.071840	0.000000
C	-4.282867	-0.663593	0.000000
H	-4.565679	0.391874	0.000000
H	-5.054533	-1.435259	0.000000

COMPLEX P

opt

Cr	0.0069	-0.0158	0.1721
C	-0.1766	-0.0254	2.0652
C	1.9003	0.0583	0.3037
C	-1.8745	-0.0701	-0.0637
O	3.0574	0.1036	0.3440
O	-0.2804	-0.0243	3.2194
O	-3.0218	-0.1026	-0.2309
C	-0.0483	1.8779	0.1623
C	0.0515	-1.9152	0.1990
O	-0.0865	3.0356	0.1716
O	0.0697	-3.0719	0.2521
C	0.2469	-0.0093	-1.8120
O	0.6240	1.0994	-2.4351
C	0.7960	1.1725	-3.8912
H	0.5969	2.2197	-4.1388
H	1.8324	0.9131	-4.1336
H	0.0987	0.5007	-4.4022
C	0.1123	-1.2206	-2.6569
C	-1.1475	-1.7606	-2.9437
C	-1.2512	-2.9309	-3.6917
C	-0.1044	-3.5872	-4.1359
C	1.1524	-3.0623	-3.8362
C	1.2639	-1.8797	-3.1103
H	-2.0470	-1.2634	-2.5801
H	-2.2374	-3.3387	-3.9165
H	-0.1891	-4.5133	-4.7050
H	2.0545	-3.5794	-4.1652
H	2.2494	-1.4820	-2.8612

Cs

Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.899400
C	1.902000	0.000000	0.000000
O	0.000000	0.000000	3.058100
O	3.060900	0.000000	0.000000
C	0.000000	1.894500	0.000000
O	0.000000	3.052900	0.000000
C	0.000000	0.000000	-1.899400
O	0.000000	0.000000	-3.058100
C	0.000000	-1.900100	0.000000
O	0.000000	-3.058200	0.000000
C	-1.998600	-0.000000	0.000000
C	-2.740100	-1.284316	0.000000
O	-2.661850	1.148783	0.000000
C	-4.129850	1.148783	0.000000
H	-4.677000	2.096474	0.000000

H	-4.677000	0.674937	-0.820725
H	-4.677000	0.674937	0.820725
C	-3.090650	-1.891486	1.214341
C	-3.090650	-1.891486	-1.214341
C	-3.786700	-3.097080	1.214341
C	-3.786700	-3.097080	-1.214341
C	-4.139650	-3.708407	0.000000
H	-2.818100	-1.419416	2.158482
H	-2.818100	-1.419416	-2.158482
H	-4.059250	-3.569150	2.158482
H	-4.059250	-3.569150	-2.158482
H	-4.684750	-4.652548	0.000000

COMPLEX Q

opt

C	-0.5674	-0.2045	0.4994
Cr	-0.3382	-0.1228	2.3847
C	-0.0062	-0.0440	4.2450
C	1.3111	-1.0513	2.1921
C	-2.0882	0.8466	2.4923
C	-1.2690	-1.7630	2.6177
C	0.5067	1.5626	2.1678
O	-0.6906	-0.2451	-0.6503
O	2.3167	-1.6134	2.0714
O	-1.8344	-2.7636	2.7557
O	1.0035	2.5999	2.0415
O	0.2434	-0.0112	5.3784
O	-2.3183	1.8571	1.6361
H	-3.2022	2.2741	1.8232
C	-3.2795	0.5582	3.3198
C	-4.5555	0.5596	2.7193
C	-5.6974	0.3308	3.4800
C	-5.5898	0.1213	4.8542
C	-4.3324	0.1127	5.4570
C	-3.1846	0.3100	4.6966
H	-4.6465	0.6870	1.6384
H	-6.6749	0.3118	2.9974
H	-6.4852	-0.0414	5.4549
H	-4.2418	-0.0471	6.5318
H	-2.2129	0.3130	5.1824

Cs

Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.891300
C	1.902500	0.000000	0.000000
O	0.000000	0.000000	3.052300
O	3.060800	0.000000	0.000000
C	0.000000	1.897800	0.000000
O	0.000000	3.054800	0.000000
C	0.000000	0.000000	-1.891300
O	0.000000	0.000000	-3.052300
C	0.000000	-1.900200	0.000000
O	0.000000	-3.057700	0.000000
C	-2.003500	-0.000000	0.000000
C	-2.742950	-1.280765	0.000000
O	-2.675650	1.164198	0.000000
H	-3.670750	1.164198	0.000000

C	-3.093500	-1.887935	1.214341
C	-3.093500	-1.887935	-1.214341
C	-3.788950	-3.092490	1.214341
C	-3.788950	-3.092490	-1.214341
C	-4.146750	-3.712218	0.000000
H	-2.820850	-1.415692	2.158828
H	-2.820850	-1.415692	-2.158828
H	-4.061600	-3.564734	2.158828
H	-4.061600	-3.564734	-2.158828
H	-4.692050	-4.656705	0.000000

COMPLEX R

opt

Cr	0.0064	-0.0089	0.1963
C	-0.1743	-0.0438	2.0741
C	1.8944	0.0510	0.3090
C	-1.8685	-0.0661	-0.0648
O	3.0540	0.0982	0.3306
O	-0.2703	-0.0491	3.2309
O	-3.0149	-0.0970	-0.2439
C	-0.0746	1.8654	0.2277
C	0.0492	-1.9143	0.2007
O	-0.1217	3.0300	0.2179
O	0.0625	-3.0704	0.2520
C	0.2576	0.0204	-1.8521
N	0.6306	1.0867	-2.5392
H	0.7867	1.9430	-2.0001
C	0.8467	1.2209	-3.9853
H	0.5570	2.2360	-4.2847
H	1.9051	1.0603	-4.2355
H	0.2332	0.4889	-4.5224
C	0.1140	-1.2129	-2.6627
C	-1.1469	-1.7529	-2.9445
C	-1.2550	-2.9360	-3.6720
C	-0.1111	-3.6040	-4.1072
C	1.1468	-3.0788	-3.8141
C	1.2613	-1.8863	-3.1043
H	-2.0450	-1.2450	-2.5923
H	-2.2434	-3.3421	-3.8906
H	-0.1998	-4.5371	-4.6641
H	2.0476	-3.6012	-4.1382
H	2.2479	-1.4865	-2.8629

Cs

Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.893900
C	1.886800	0.000000	0.000000
O	0.000000	0.000000	3.054600
O	3.047600	0.000000	0.000000
C	0.000000	1.887630	0.000000
O	0.000000	3.053230	0.000000
C	0.000000	0.000000	-1.893900
O	0.000000	0.000000	-3.054600
C	0.000000	-1.905900	0.000000
O	0.000000	-3.063200	0.000000
C	-2.064000	-0.000000	0.000000
C	-2.805400	-1.284142	0.000000

N	-2.725100	1.145059	0.000000
C	-4.193400	1.145059	0.000000
H	-4.742050	2.095348	0.000000
H	-4.742050	0.669914	-0.822975
H	-4.742050	0.669914	0.822975
C	-3.155475	-1.890490	1.212695
C	-3.155475	-1.890490	-1.212695
C	-3.852025	-3.096950	1.212695
C	-3.852025	-3.096950	-1.212695
C	-4.206700	-3.711265	0.000000
H	-2.882925	-1.418420	2.156836
H	-2.882925	-1.418420	-2.156836
H	-4.124575	-3.569021	2.156836
H	-4.124575	-3.569021	-2.156836
H	-4.751800	-4.655406	0.000000
H	-2.152598	1.993827	0.000000

COMPLEX S

opt

Cr	-0.0029	-0.0122	0.2069
C	-0.1318	-0.0367	2.0944
C	1.8925	-0.0124	0.2706
C	-1.8867	-0.0092	-0.0058
O	3.0520	-0.0011	0.2755
O	-0.1979	-0.0337	3.2522
O	-3.0333	-0.0015	-0.1798
C	-0.0030	1.8622	0.2197
C	-0.0113	-1.9197	0.2138
O	0.0048	3.0268	0.1741
O	-0.0266	-3.0752	0.2686
C	0.1394	0.0130	-1.8274
N	0.2785	1.0862	-2.5893
H	0.3244	2.0230	-2.1822
H	0.3399	1.0151	-3.6114
C	0.1047	-1.2301	-2.6379
C	-1.1195	-1.7781	-3.0383
C	-1.1436	-2.9470	-3.7955
C	0.0463	-3.5808	-4.1511
C	1.2657	-3.0388	-3.7477
C	1.2994	-1.8661	-2.9961
H	-2.0516	-1.2907	-2.7497
H	-2.1016	-3.3656	-4.1059
H	0.0229	-4.4997	-4.7375
H	2.2005	-3.5315	-4.0171
H	2.2532	-1.4488	-2.6694

Cs

Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.895800
C	1.892100	0.000000	0.000000
O	0.000000	0.000000	3.055600
O	3.051800	0.000000	0.000000
C	0.000000	1.874400	0.000000
O	0.000000	3.039900	0.000000
C	0.000000	0.000000	-1.895800
O	0.000000	0.000000	-3.055600
C	0.000000	-1.907500	0.000000

O	0.000000	-3.064400	0.000000
C	-2.039400	-0.000000	0.000000
C	-2.781600	-1.285528	0.000000
N	-2.701150	1.146185	0.000000
H	-3.727550	1.146185	0.000000
C	-3.131525	-1.891616	1.212176
C	-3.131525	-1.891616	-1.212176
C	-3.827975	-3.097903	1.212176
C	-3.827975	-3.097903	-1.212176
C	-4.179700	-3.707108	0.000000
H	-2.858875	-1.419372	2.156663
H	-2.858875	-1.419372	-2.156663
H	-4.100625	-3.570146	2.156663
H	-4.100625	-3.570146	-2.156663
H	-4.725000	-4.651596	0.000000

COMPLEX T

opt

C	-0.5734	-0.3062	0.4986
Cr	-0.3254	-0.1655	2.3803
C	-0.0556	0.0001	4.2495
C	1.4092	-0.9595	2.1979
C	-2.1219	0.6489	2.4533
C	-1.1133	-1.8649	2.6837
C	0.3736	1.5848	2.1043
O	-0.7175	-0.3666	-0.6476
O	2.4511	-1.4507	2.0904
O	-1.6123	-2.8886	2.8883
O	0.7840	2.6535	1.9403
O	0.1184	0.0806	5.3919
H	-2.3666	1.3576	1.6441
C	-3.2807	0.5071	3.2992
C	-4.4917	1.1320	2.9052
C	-5.6470	1.0120	3.6630
C	-5.6207	0.2831	4.8531
C	-4.4378	-0.3331	5.2725
C	-3.2880	-0.2326	4.5049
H	-4.5045	1.7071	1.9775
H	-6.5699	1.4896	3.3329
H	-6.5236	0.1956	5.4588
H	-4.4185	-0.8948	6.2068
H	-2.3775	-0.7185	4.8451

Cs

Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.895800
C	1.916400	0.000000	0.000000
O	0.000000	0.000000	3.054200
O	3.073300	0.000000	0.000000
C	0.000000	1.904800	0.000000
O	0.000000	3.061300	0.000000
C	0.000000	0.000000	-1.895800
O	0.000000	0.000000	-3.054200
C	0.000000	-1.897600	0.000000
O	0.000000	-3.054700	0.000000
C	-1.973800	-0.000000	0.000000
C	-2.694650	-1.248549	0.000000

H	-2.525350	0.955313	0.000000
C	-3.048275	-1.861045	1.224993
C	-3.048275	-1.861045	-1.224993
C	-3.741325	-3.061443	1.224993
C	-3.741325	-3.061443	-1.224993
C	-4.103600	-3.688922	0.000000
H	-2.776600	-1.390490	2.166103
H	-2.776600	-1.390490	-2.166103
H	-4.013900	-3.533557	2.169220
H	-4.013900	-3.533557	-2.169220
H	-4.649000	-4.633582	0.000000

COMPLEX U

opt

Cr	0.122534	-0.010194	0.175652
C	-0.078174	-0.062761	2.068885
C	1.773727	-0.947241	0.300800
C	-1.513991	0.934825	-0.027911
O	2.779593	-1.515570	0.366611
O	-0.195818	-0.093480	3.220564
O	-2.505161	1.512692	-0.175715
C	1.023990	1.654750	0.290813
C	-0.775923	-1.676970	0.031880
O	1.569040	2.673522	0.356183
O	-1.313183	-2.699368	-0.048519
C	0.350240	0.052624	-1.809365
O	0.343092	1.208668	-2.478134
C	0.528186	1.214544	-3.927277
H	0.486619	2.269625	-4.211552
H	1.504532	0.780550	-4.173589
H	-0.280464	0.647677	-4.403574
C	0.532714	-1.118141	-2.578134
H	0.802537	-3.138440	-3.614272
C	0.677239	-2.190051	-3.135807

Cs

Cr	0.000000	0.000000	0.000000
C	1.904700	0.000000	0.000000
C	0.000000	1.903200	0.000000
O	3.061600	0.000000	0.000000
O	0.000000	3.061500	0.000000
C	0.000000	0.000000	1.896400
O	0.000000	0.000000	3.054100
C	-1.904700	0.000000	0.000000
O	-3.061600	0.000000	0.000000
C	0.000000	0.000000	-1.895800
O	0.000000	0.000000	-3.054300
C	0.000000	-2.000700	-0.000000
C	0.000000	-2.706900	-1.223174
O	0.000000	-2.668200	1.156144
C	0.000000	-4.129600	1.156144
C	0.000000	-3.315400	-2.277127
H	0.000000	-3.850100	-3.203255
H	0.820050	-4.676300	0.682688
H	0.000000	-4.676300	2.103056
H	-0.820050	-4.676300	0.682688

COMPLEX V

opt

C	-0.4160	-0.2001	0.4280
Cr	-0.3022	-0.1281	2.3240
C	-0.2192	-0.0292	4.2212
C	1.3854	-1.0236	2.2900
C	-2.0537	0.7896	2.3693
C	-1.2023	-1.7990	2.4773
C	0.5488	1.5635	2.1506
O	-0.4803	-0.2391	-0.7257
O	2.4051	-1.5696	2.2767
O	-1.7604	-2.8071	2.5753
O	1.0561	2.5956	2.0337
O	-0.1816	0.0264	5.3762
O	-2.4144	1.7294	1.4684
H	-3.3279	2.0618	1.6692
C	-3.0414	0.5264	3.3428
C	-3.8495	0.2590	4.2117
H	-4.5532	0.0172	4.9803

Cs

Cr	0.000000	0.000000	0.000000
C	1.904100	0.000000	0.000000
C	0.000000	1.910800	0.000000
O	3.060500	0.000000	0.000000
O	0.000000	3.067600	0.000000
C	0.000000	0.000000	1.900800
O	0.000000	0.000000	3.056900
C	-1.904100	0.000000	0.000000
O	-3.060500	0.000000	0.000000
C	0.000000	0.000000	-1.901600
O	0.000000	0.000000	-3.058500
C	0.000000	-1.977900	-0.000000
C	0.000000	-2.684100	-1.223174
O	0.000000	-2.653350	1.169914
H	0.000000	-3.645950	1.169914
C	0.000000	-3.292600	-2.277127
H	0.000000	-3.827300	-3.203255

COMPLEX W

opt

Cr	0.0358	-0.0049	0.1833
C	-0.2021	-0.0475	2.0535
C	1.9238	0.0673	0.3663
C	-1.8365	-0.0862	-0.1365
O	3.0787	0.1168	0.4452
O	-0.3316	-0.0608	3.2066
O	-2.9769	-0.1370	-0.3311
C	-0.0634	1.8668	0.2404
C	0.0937	-1.9068	0.1921
O	-0.1269	3.0307	0.2590
O	0.1132	-3.0630	0.2470
C	0.3700	0.0655	-1.8550
N	0.4999	1.1812	-2.5675
H	0.4174	2.0600	-2.0532
C	0.8271	1.2938	-3.9891

H	0.4803	2.2675	-4.3537
H	1.9142	1.2139	-4.1372
H	0.3265	0.4938	-4.5473
C	0.5308	-1.1321	-2.5852
H	0.8006	-3.1692	-3.5845
C	0.6753	-2.2104	-3.1276

Cs

Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.901200
C	1.885800	0.000000	0.000000
O	0.000000	0.000000	3.059200
O	3.046200	0.000000	0.000000
C	0.000000	1.875200	0.000000
O	0.000000	3.041000	0.000000
C	0.000000	0.000000	-1.901200
O	0.000000	0.000000	-3.059200
C	0.000000	-1.902800	0.000000
O	-0.814936	-2.725082	0.000000
C	-2.066700	-0.000000	0.000000
C	-2.772600	-1.222655	0.000000
N	-2.731800	1.151987	0.000000
C	-4.194900	1.151987	0.000000
H	-4.742900	0.677405	0.822000
H	-4.742900	2.101151	0.000000
H	-4.742900	0.677405	-0.822000
H	-2.221000	2.036719	0.000000
C	-3.380450	-2.275482	0.000000
H	-3.915200	-3.201696	0.000000

COMPLEX X

opt

Cr	0.0483	-0.0071	0.1907
C	-0.2168	-0.0594	2.0620
C	1.9336	0.0878	0.4107
C	-1.8226	-0.0899	-0.1470
O	3.0839	0.1636	0.5181
O	-0.3652	-0.0806	3.2117
O	-2.9587	-0.1313	-0.3638
C	-0.0559	1.8645	0.2234
C	0.1220	-1.9095	0.1831
O	-0.1164	3.0278	0.2031
O	0.1552	-3.0655	0.2242
C	0.3746	0.0609	-1.8300
N	0.5444	1.1675	-2.5534
H	0.5049	2.0857	-2.1114
H	0.7237	1.1373	-3.5612
C	0.4614	-1.1252	-2.5909
H	0.5994	-3.1190	-3.6963
C	0.5349	-2.1812	-3.1872

Cs

Cr	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.902900
C	1.890700	0.000000	0.000000
O	0.000000	0.000000	3.060200
O	3.050100	0.000000	0.000000
C	0.000000	1.874800	0.000000

O	0.000000	3.039800	0.000000
C	0.000000	0.000000	-1.902900
O	0.000000	0.000000	-3.060200
C	0.000000	-1.903800	0.000000
O	0.000000	-3.061000	0.000000
C	-2.048000	-0.000000	0.000000
C	-2.753950	-1.222741	0.000000
N	-2.714450	1.154325	0.000000
H	-3.738550	1.154325	0.000000
H	-2.204550	2.037498	0.000000
C	-3.361450	-2.274962	0.000000
H	-3.895950	-3.200743	0.000000

COMPLEX Y

opt

C	-0.4290	-0.1870	0.4386
Cr	-0.2978	-0.1376	2.3364
C	-0.2072	-0.0574	4.2401
C	1.4089	-1.0192	2.2625
C	-2.0340	0.7770	2.3982
C	-1.1916	-1.8149	2.5170
C	0.5456	1.5595	2.1460
O	-0.4974	-0.1990	-0.7152
O	2.4342	-1.5501	2.2197
O	-1.7496	-2.8186	2.6335
O	1.0477	2.5915	2.0103
O	-0.1748	-0.0125	5.3932
H	-2.2883	1.5675	1.6734
C	-3.0565	0.5509	3.2991
C	-3.9298	0.3176	4.1233
H	-4.6949	0.1152	4.8425

Cs

Cr	0.000000	0.000000	0.000000
C	1.909100	0.000000	0.000000
C	0.000000	1.922400	0.000000
O	3.063400	0.000000	0.000000
O	0.000000	3.077800	0.000000
C	0.000000	0.000000	1.903000
O	0.000000	0.000000	3.058900
C	-1.909100	0.000000	0.000000
O	-3.063400	0.000000	0.000000
C	0.000000	0.000000	-1.907500
O	0.000000	0.000000	-3.061900
C	0.000000	-1.963300	-0.000000
C	0.000000	-2.654000	-1.196327
H	0.000000	-2.514400	0.954533
C	0.000000	-3.265650	-2.255736
H	0.000000	-3.800350	-3.181864