

Complexe III

C	3.723	-2.760	-1.259
C	2.227	-2.551	-0.851
C	1.626	-2.142	-2.214
C	2.558	-0.924	-2.385
C	3.955	-1.628	-2.320
C	2.216	-1.233	-0.073
C	2.400	-0.210	-1.041
Co	0.571	0.086	-0.041
C	-0.445	-1.526	0.474
C	-1.017	-0.913	-0.585
Co	-1.586	-0.122	1.162
C	-1.087	0.019	2.867
O	-0.788	0.040	3.995
C	1.216	1.100	1.260
O	1.631	1.822	2.080
C	-3.155	-0.868	1.294
O	-4.206	-1.374	1.379
P	-2.331	1.958	0.518
C	-1.445	2.654	-0.827
P	-0.017	1.814	-1.402
C	-0.282	1.394	-3.223
C	-2.388	3.200	1.937
C	-4.153	2.042	0.048
C	1.320	3.118	-1.651
H	3.870	-3.755	-1.703
H	4.400	-2.676	-0.400
H	1.776	-3.416	-0.351
H	1.776	-2.908	-2.989
H	0.573	-1.869	-2.156
H	2.411	-0.314	-3.283
H	4.226	-2.052	-3.298
H	4.750	-0.931	-2.026
H	2.657	-1.219	0.922
H	2.996	0.681	-0.850
H	-0.153	-2.512	0.819
H	-1.598	-1.170	-1.465
H	-1.825	3.540	-1.344
H	0.631	0.995	-3.684
H	-1.073	0.640	-3.290
H	-0.603	2.288	-3.778
H	-2.734	4.181	1.582
H	-3.051	2.849	2.741
H	-1.374	3.307	2.338
H	-4.418	3.055	-0.286

H	-4.336	1.342	-0.775
H	-4.797	1.767	0.895
H	0.933	3.960	-2.242
H	1.628	3.494	-0.668
H	2.197	2.698	-2.164

Cobaltacycle IV

C	-2.408	-2.416	-1.035
C	-2.570	-2.512	0.497
C	-1.533	-1.466	1.013
C	-1.559	-0.361	-0.098
C	-2.635	-0.887	-1.077
C	-3.983	-1.908	0.691
C	-4.029	-0.779	-0.395
Co	0.324	-0.039	-0.746
C	0.111	-0.634	-2.355
O	0.030	-1.098	-3.426
C	-0.124	-2.008	1.133
C	0.800	-1.660	0.126
Co	1.204	-0.409	1.617
C	2.034	-1.129	2.973
O	2.579	-1.611	3.896
C	0.204	0.898	2.241
O	-0.434	1.774	2.697
P	0.807	2.161	-1.066
P	2.914	0.426	0.482
C	2.238	1.063	-1.053
C	0.864	2.928	-2.770
C	1.027	3.695	-0.005
C	4.053	1.700	1.276
C	4.217	-0.762	-0.141
H	-3.170	-2.989	-1.587
H	-1.414	-2.713	-1.381
H	-2.450	-3.511	0.938
H	-1.878	-1.085	1.986
H	-1.854	0.618	0.298
H	-2.614	-0.426	-2.072
H	-4.763	-2.661	0.510
H	-4.126	-1.521	1.709
H	-4.840	-0.960	-1.117
H	-4.189	0.217	0.040
H	0.016	-2.915	1.735
H	1.598	-2.339	-0.186
H	2.865	1.051	-1.951
H	1.760	3.548	-2.909
H	0.863	2.124	-3.515
H	-0.027	3.547	-2.932
H	1.941	4.241	-0.278
H	0.157	4.354	-0.134
H	1.072	3.400	1.047
H	3.452	2.554	1.612
H	4.536	1.257	2.157
H	4.823	2.056	0.575
H	4.919	-0.262	-0.823
H	4.772	-1.177	0.709
H	3.724	-1.582	-0.673

III->IV

4.659113	-1.654358	- .050525
3.238340	-1.648017	- .696064
3.315666	- .362935	-1.550253
3.658244	.547238	- .352945
4.967630	- .132147	.154627
2.263402	-1.247167	.427136
2.569884	.180400	.662202
.594519	.166421	.412834
.520610	-1.648132	- .511133
.063316	- .592383	-1.280017
-1.376705	-1.177891	- .100308
-1.743676	-1.791374	1.523740
-1.984449	-2.247569	2.572638
.189194	.442764	2.113849
- .120975	.730086	3.203177
-2.275195	-2.257302	-1.136177
-2.884975	-2.976853	-1.830711
-2.613672	.743067	- .343910
-1.690122	2.230498	- .569130
.041715	2.171336	- .321165
.922304	2.785148	-1.870348
-3.857634	1.012801	1.046773
-3.841634	.686953	-1.769505
.540758	3.587477	.813306
.818100	-2.667963	- .738260
2.787703	.486876	1.688542
2.202842	-1.931635	1.275163
.032987	- .369138	-2.343435
3.768236	1.617754	- .564836
2.992377	-2.575712	-1.226365
5.835622	.179619	- .444967
5.179147	.118269	1.201924
5.385332	-2.119006	- .732055
4.678572	-2.221247	.889031
4.115340	- .403911	-2.303986
2.369294	- .106594	-2.027669
-4.437891	1.932734	.883971
-4.545061	.158910	1.127309
-3.303372	1.107289	1.987199
-4.370284	1.646385	-1.865130
-3.289992	.495655	-2.696813
-4.577304	- .115560	-1.623546
.152061	4.543787	.434942
.119467	3.406010	1.808124
1.634895	3.654161	.896811
2.008294	2.844593	-1.716647
.715789	2.086332	-2.687578
.545181	3.778136	-2.153945
-2.196966	3.165803	- .823931