Table S1: Cartesian coordinates of UB3LYP/TZV optimized geometry of $[Co([3^5]adz)]^{2+}$ from a Gaussian 98 Rev. A7 calculation.

Atom	X	Y	Z
Co	0.0000000	0.0000000	0.5677699
C	0.0000000	0.0000000	-2.7099482
H	0.2193800	0.8349460	-3.3776461
H	-0.2193800	-0.8349460	-3.3776461
C	-1.3201250	0.2763170	-1.9479581
C	1.3201250	-0.2763170	-1.9479581
H	-2.0016961	0.7950440	-2.6290351
H	-1.7985660	-0.6685570	-1.6997871
H	2.0016961	-0.7950440	-2.6290351
H	1.7985660	0.6685570	-1.6997871
N	-1.2321230	1.0637770	-0.6556091
N	1.2321230	-1.0637770	-0.6556091
C	-0.7060450	2.4684291	-0.9053922
C	0.7060450	-2.4684291	-0.9053922
H	-1.5228040	3.0672820	-1.3168961
H	0.0595110	2.4076600	-1.6772171
H	1.5228040	-3.0672820	-1.3168961
H	-0.0595110	-2.4076600	-1.6772171
C	-0.1186820	3.1709459	0.3313869
C	0.1186820	-3.1709459	0.3313869
H	0.0000000	4.2237992	0.0649279
H	-0.8254160	3.1695931	1.1658239
H	0.0000000	-4.2237992	0.0649279
H	0.8254160	-3.1695931	1.1658239
C	1.2561740	2.6691511	0.7948349
C	-1.2561740	-2.6691511	0.7948349
H	1.7179360	3.4078860	1.4528599
H	1.9175810	2.5488670	-0.0615691
H	-1.7179360	-3.4078860	1.4528599
H	-1.9175810	-2.5488670	-0.0615691
N	1.1999810	1.3428090	1.5347838
N	-1.1999810	-1.3428090	1.5347838
H	0.8069960	1.5452650	2.4565378
H	-0.8069960	-1.5452650	2.4565378
C	2.5783110	0.7452830	1.7713959
C	-2.5783110	-0.7452830	1.7713959
H	3.2312651	1.5232350	2.1731328
H	2.4684410	-0.0148570	2.5471958
H	-3.2312651	-1.5232350	2.1731328
H	-2.4684410	0.0148570	2.5471958
C	3.2282550	0.1340650	0.5221459
C	-3.2282550	-0.1340650	0.5221459
H	4.2539930	-0.1172160	0.8044989
H	3.3379071	0.8817520	-0.2639661
H	-4.2539930	0.1172160	0.8044989
H	-3.3379071	-0.8817520	-0.2639661
C	2.6161110	-1.1672291	-0.0235231
C	-2.6161110	1.1672291	-0.0235231
H	2.5463841	-1.8953249	0.7840999
H	3.2912540	-1.5886050	-0.7739361
H	-2.5463841	1.8953249	0.7840999
H	-3.2912540	1.5886050	-0.7739361