

Supporting Information

Optimized Geometry for model of $[\text{Au}([\text{9}] \text{aneS}_2\text{O})_2]^{2+}$

Au	0.00000	0.00000	0.00000
S	1.72367	1.84277	0.00000
S	1.72367	-1.87121	0.00000
S	-1.72367	1.87121	0.00000
S	-1.72367	-1.84277	0.00000
O	-0.04978	-1.14353	2.63782
O	0.04978	1.14353	-2.63782
H	1.89785	-0.66975	2.87731
H	1.28996	4.00798	0.93648
H	2.91127	-2.68757	1.91070
H	1.41074	-2.10695	3.79552
H	2.94563	2.71738	-1.88441
H	2.68958	0.96219	-1.96173
H	0.65364	3.89427	-0.71213
H	-0.60878	2.75595	1.87958
H	1.34956	-3.50231	1.74029
H	-1.24139	4.06356	0.86602
H	0.64014	3.16199	-2.69041
H	1.49697	2.08132	-3.80160
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H	-0.64014	-3.16199	2.69041
H	1.24139	-4.06356	-0.86602
H	-1.34956	3.50231	-1.74029
H	-0.65364	-3.89427	0.71213
H	0.60878	-2.75595	-1.87958
H	-2.68958	-0.96219	1.96173
H	-2.94563	-2.71738	1.88441
H	-1.41074	2.10695	-3.79552
H	-2.91127	2.68757	-1.91070
H	-1.28996	-4.00798	-0.93648
H	-1.89785	0.66975	-2.87731
C	1.29734	-1.58694	2.82886
C	0.71110	3.37372	0.25059
C	1.83926	-2.52067	1.73721
C	2.18904	1.92568	-1.79205
C	-0.67024	3.12476	0.84687
C	1.05979	2.14894	-2.79051
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C	0.67024	-3.12476	-0.84687
C	-2.18904	-1.92568	1.79205
C	-1.83926	2.52067	-1.73721
C	-0.71110	-3.37372	-0.25059
C	-1.29734	1.58694	-2.82886

Total Energy: -7.63463369 a.u.