Assignment 3

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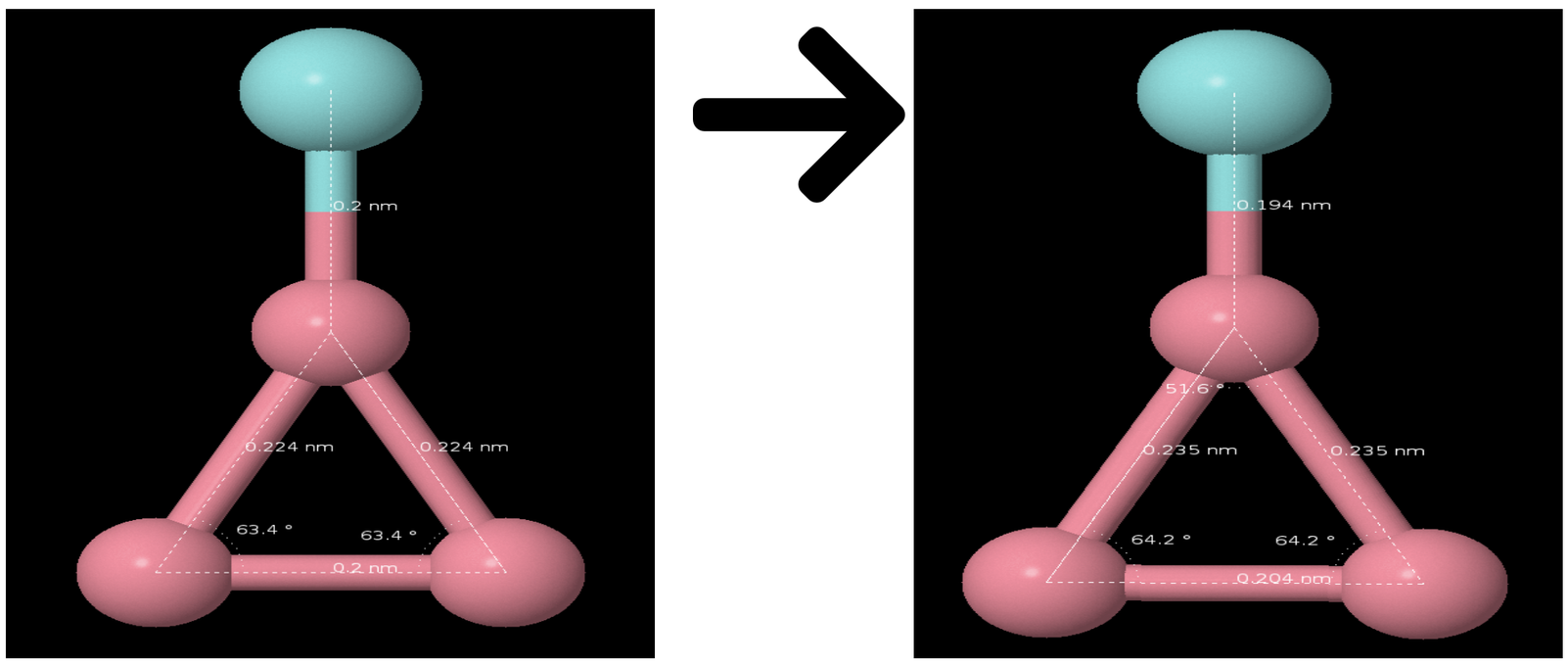
I tried about 15 configuration. The below six are the only that converged. To get the raw data related to these configurations, click here.

Configuration 1



Initial Geometry

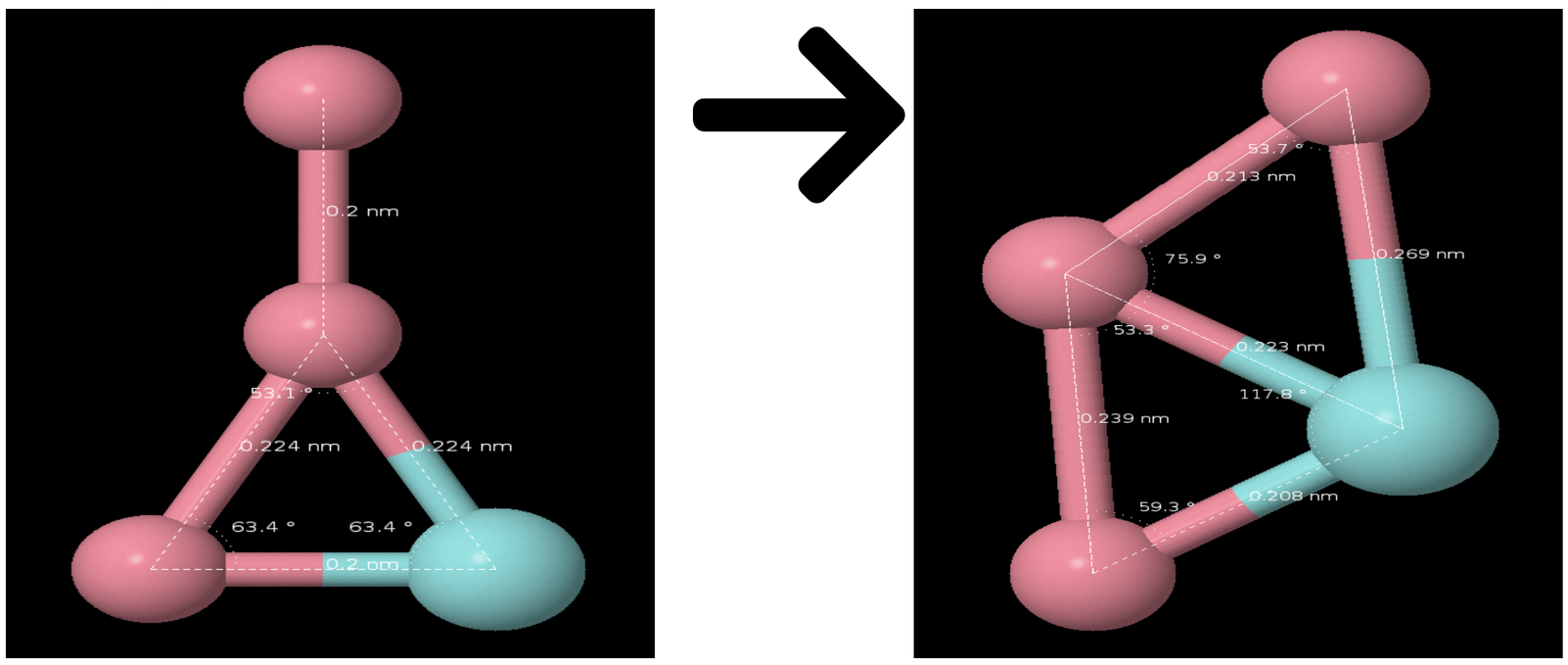
atom	-1	0	0	**Co**
atom	1	0	0	**Co**
atom	0	2	0	**Co**
atom	0	4	0	**Zr**

Final Geometry

atom	-1.02195984	-0.04171919	-0.00000000	**Co**
atom	1.02195984	-0.04171915	-0.00000000	**Co**
atom	-0.00000003	2.07303559	0.00000002	**Co**
atom	0.00000003	4.01040275	-0.00000001	**Zr**

Energy: -212991.530759 eV

Configuration 2



Initial Geometry

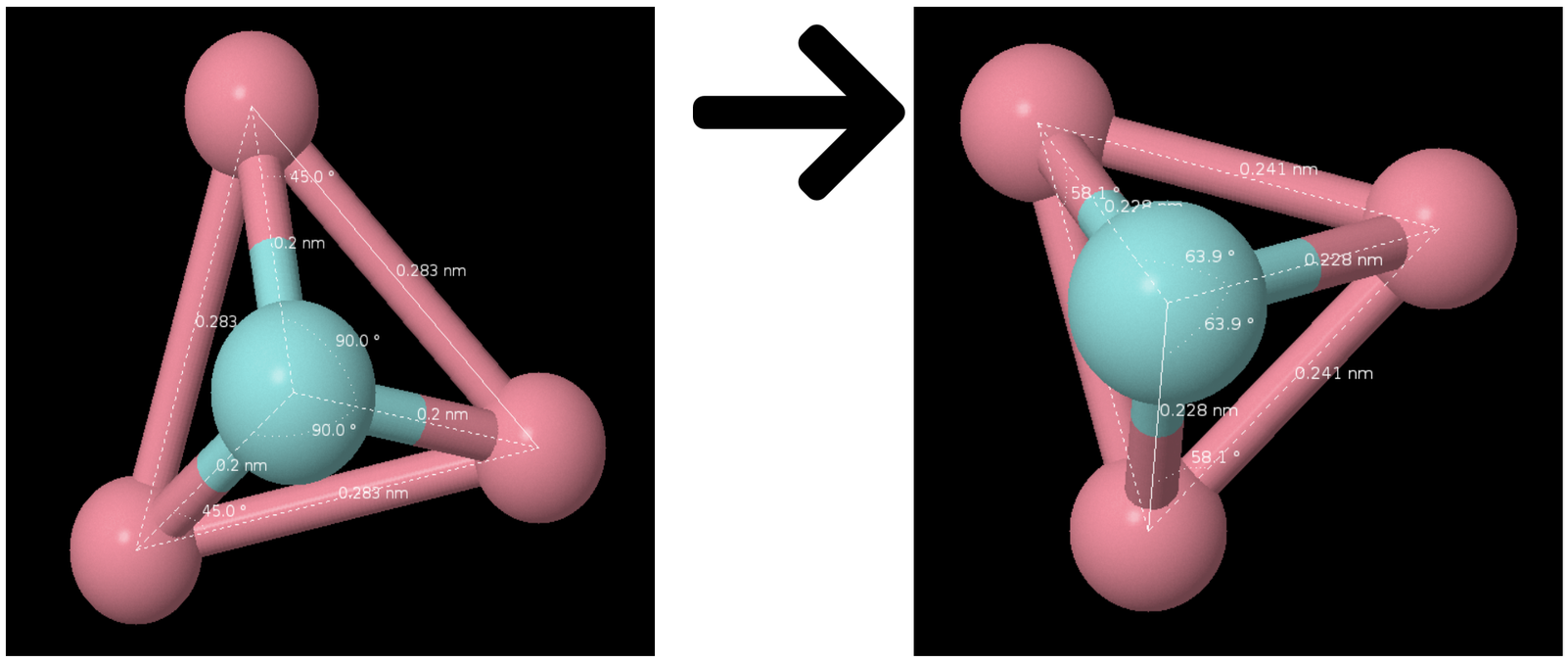
atom	-1	0	0	**Co**
atom	1	0	0	**Zr**
atom	0	2	0	**Co**
atom	0	4	0	**Co**

Final Geometry

atom	-0.74415541	-0.35114249	0.00000005	**Co**
atom	0.97367750	0.82228537	-0.00000003	**Zr**
atom	-0.89607783	2.03889434	-0.00000006	**Co**
atom	0.66655574	3.48996277	0.00000004	**Co**

Energy: -212992.883825 eV

Configuration 3



Initial Geometry

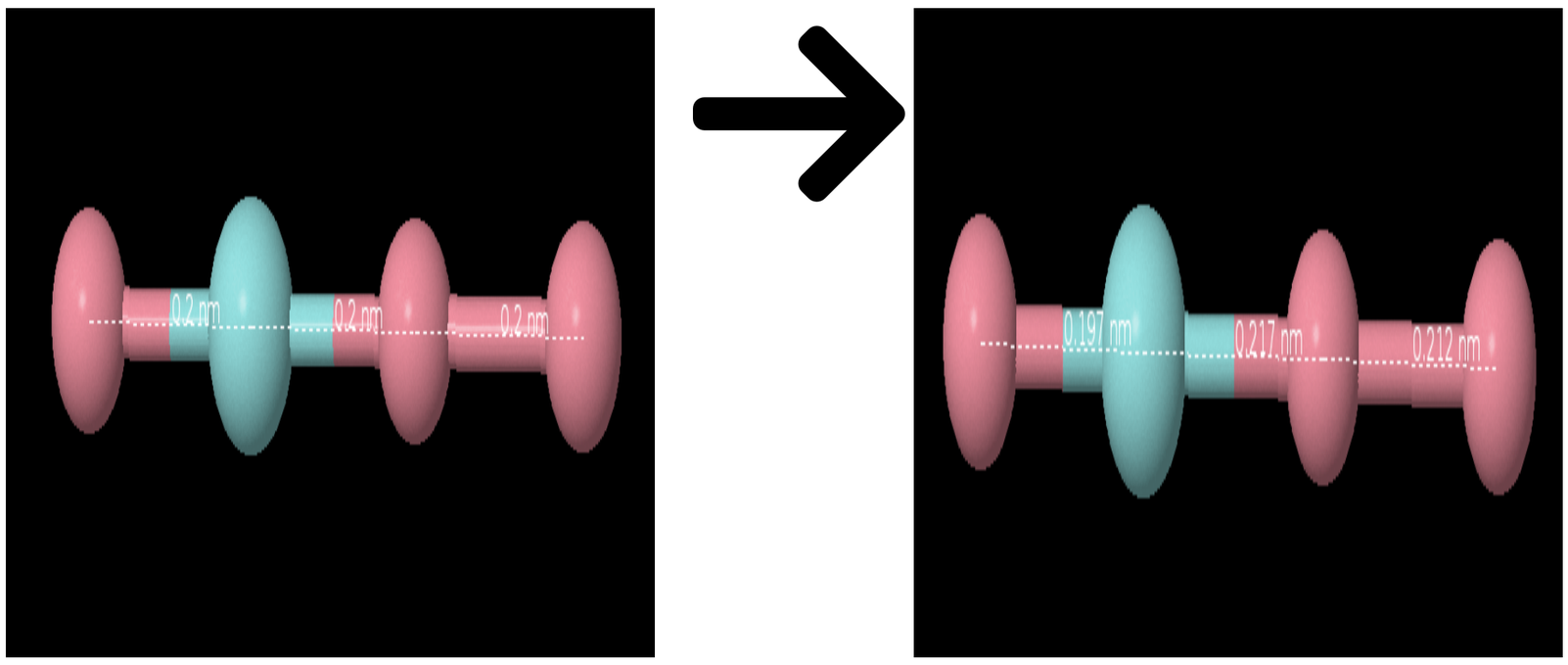
atom	0	0	0	**Zr**
atom	2	0	0	**Co**
atom	0	2	0	**Co**
atom	0	0	2	**Co**

Final Geometry

atom	-0.28221476	-0.28221486	-0.28221486	**Zr**
atom	1.89849074	0.19186199	0.19186198	**Co**
atom	0.19186202	1.89849080	0.19186207	**Co**
atom	0.19186200	0.19186207	1.89849081	**Co**

Energy: -212992.912984 eV

Configuration 4



Initial Geometry

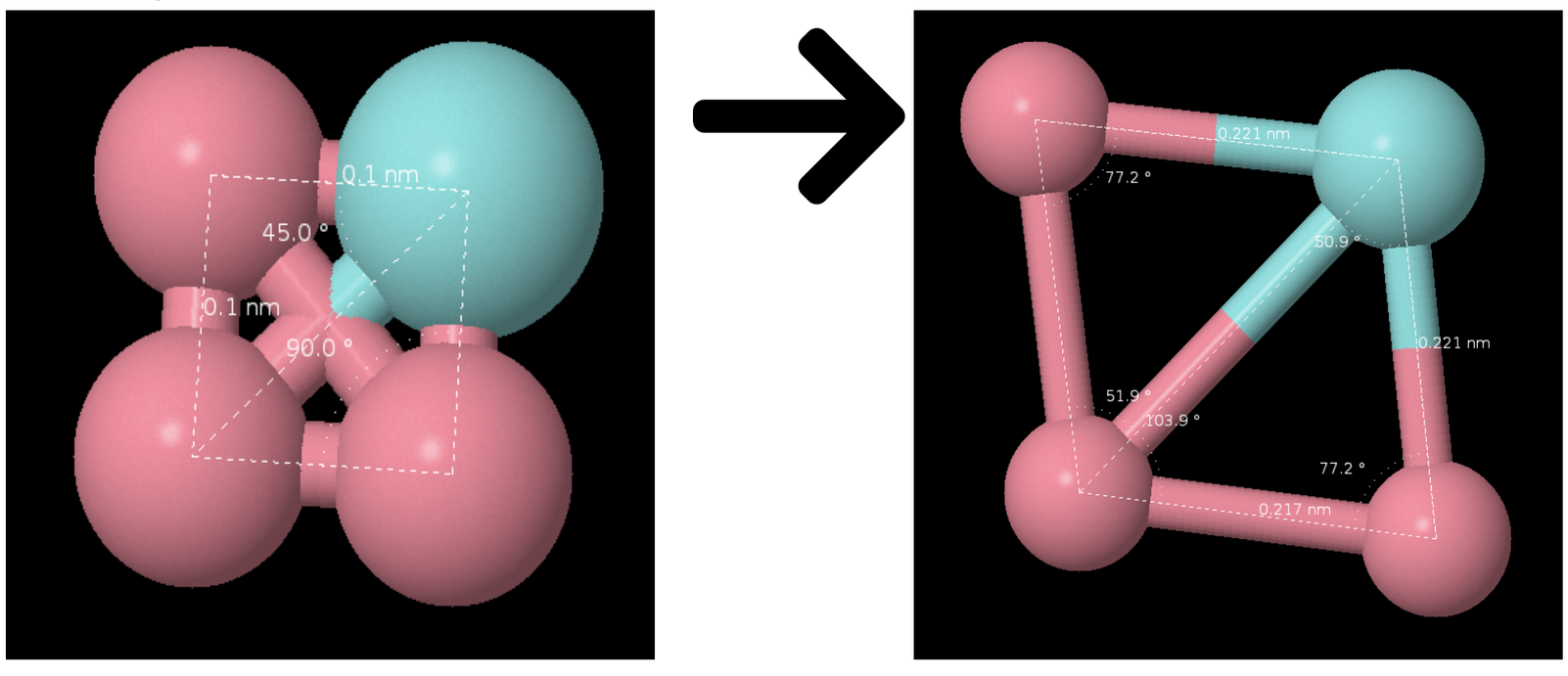
atom	0	0	0	**Co**
atom	0	0	2	**Co**
atom	0	0	4	**Zr**
atom	0	0	6	**Co**

Final Geometry

atom	0.00000001	-0.00000002	-0.16985336	**Co**
atom	-0.00000002	0.00000002	1.95213864	**Co**
atom	0.00000000	0.00000001	4.12362956	**Zr**
atom	0.00000001	-0.00000001	6.09408515	**Co**

Energy: -212990.966254 eV

Configuration 5



Initial Geometry

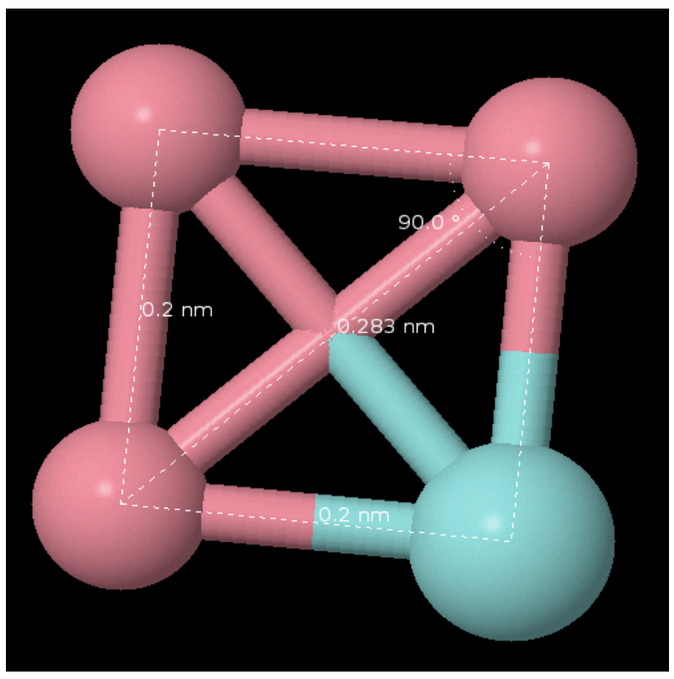
Final Geometry

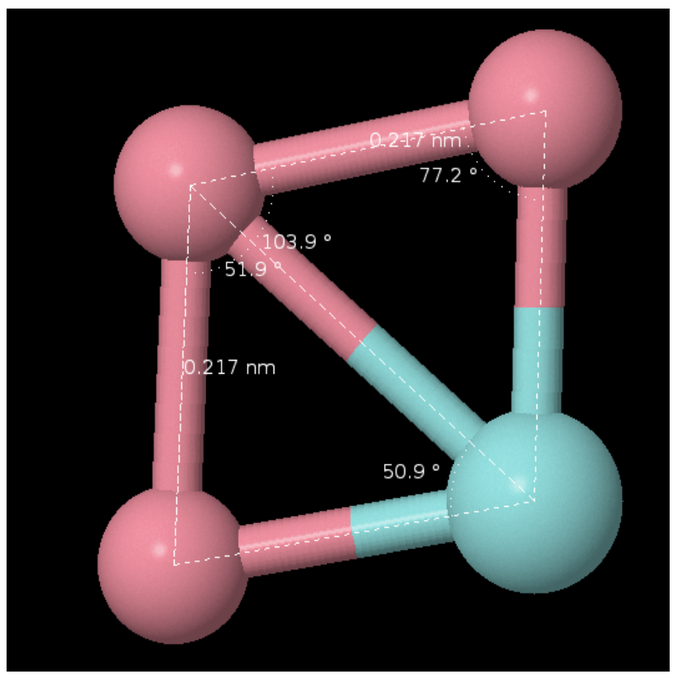
atom	0	0	0	**Co**
atom	1	1	0	**Zr**
atom	0	1	0	**Co**
atom	1	0	0	**Co**

atom	-0.45698498	-0.45698490	0.00000000	**Co**
atom	1.47449397	1.47449396	0.00000000	**Zr**
atom	-0.71922188	1.70171278	-0.00000000	**Co**
atom	1.70171289	-0.71922183	-0.00000000	**Co**

Energy: -212993.138496 eV

Configuration 6





Initial Geometry

atom	0	0	2	**Co**
atom	0	0	0	**Zr**
atom	0	2	2	**Co**
atom	0	2	0	**Co**

Final Geometry

atom	0.00000001	-0.20170932	2.21922135	**Co**
atom	-0.00000001	0.02548169	0.02548171	**Zr**
atom	-0.00000001	1.95700626	1.95700627	**Co**
atom	0.00000001	2.21922138	-0.20170932	**Co**

Energy: -212993.138417 eV