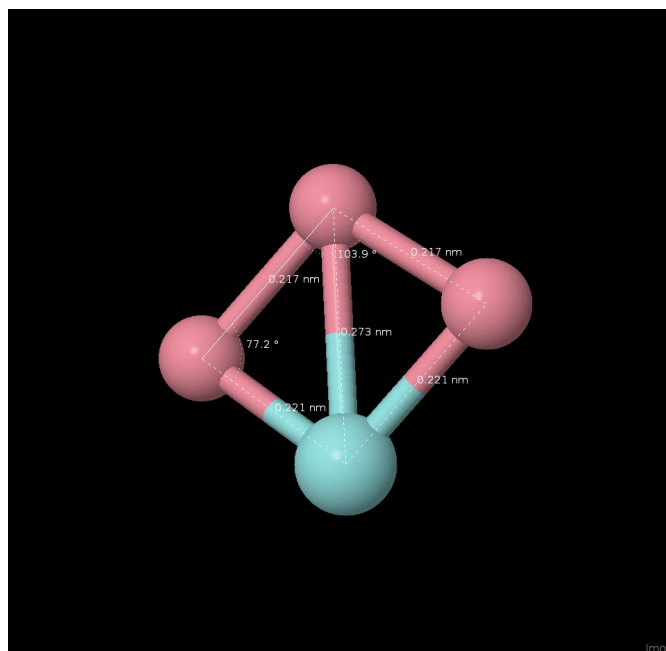
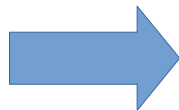
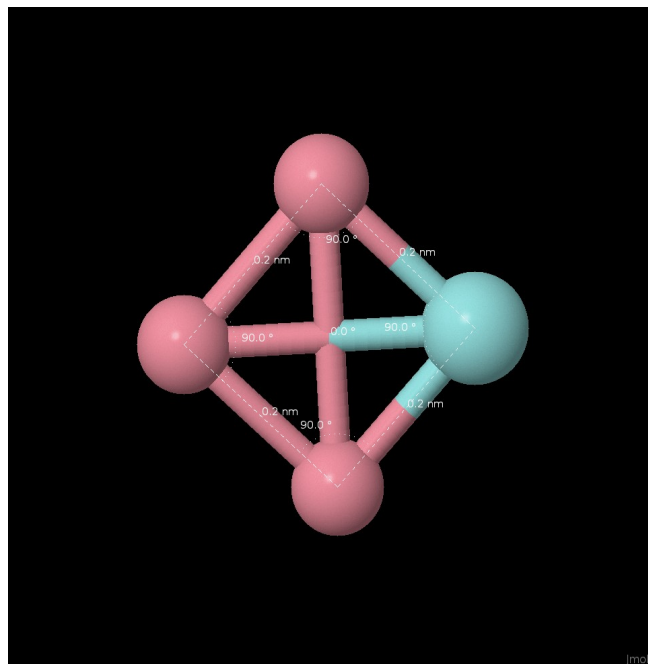


Name- Shailja Kant Tiwari  
Entry No. - 2021PHS217218  
ASSIGNMENT-3

## Structure-1



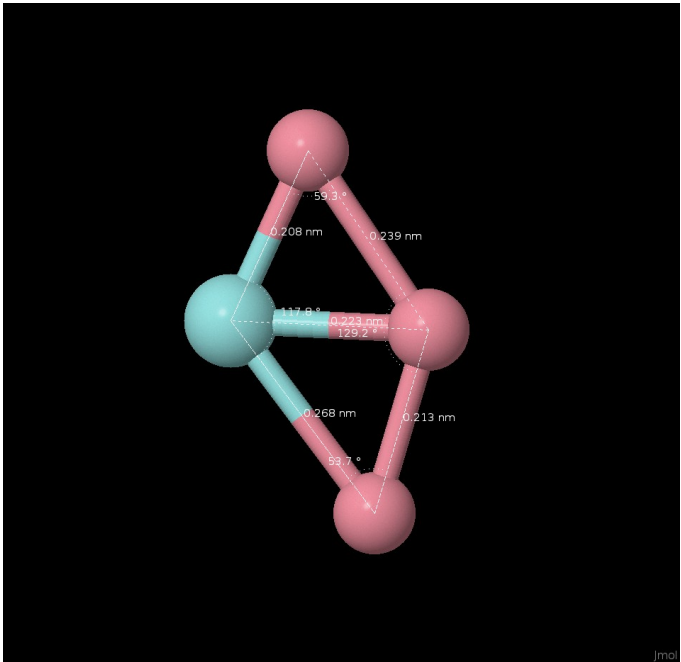
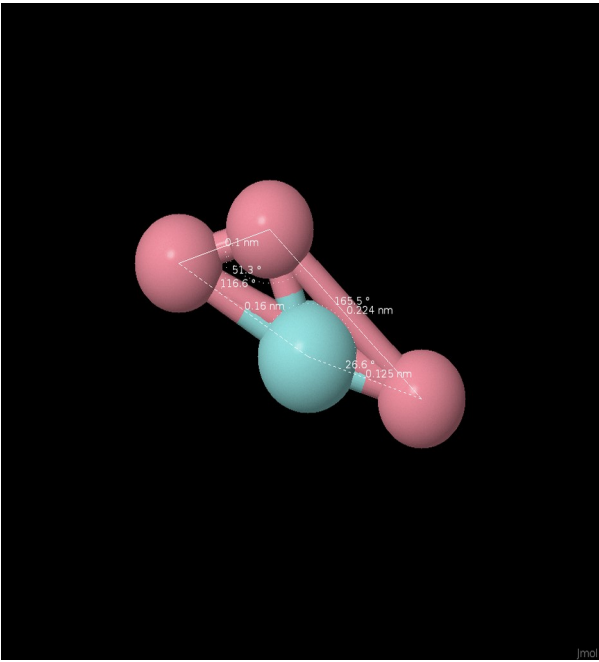
atom	0	0	0	Co
atom	0	2	0	Co
atom	2	0	0	Zr
atom	2	2	0	Co



atom	-0.21922134	-0.20170934	0.00000000	Co
atom	0.04299373	1.95700628	-0.00000000	Co
atom	1.97451829	0.02548173	-0.00000000	Zr
atom	2.20170932	2.21922132	0.00000000	Co

Energy = **-212993.138496 eV**

Structure-2



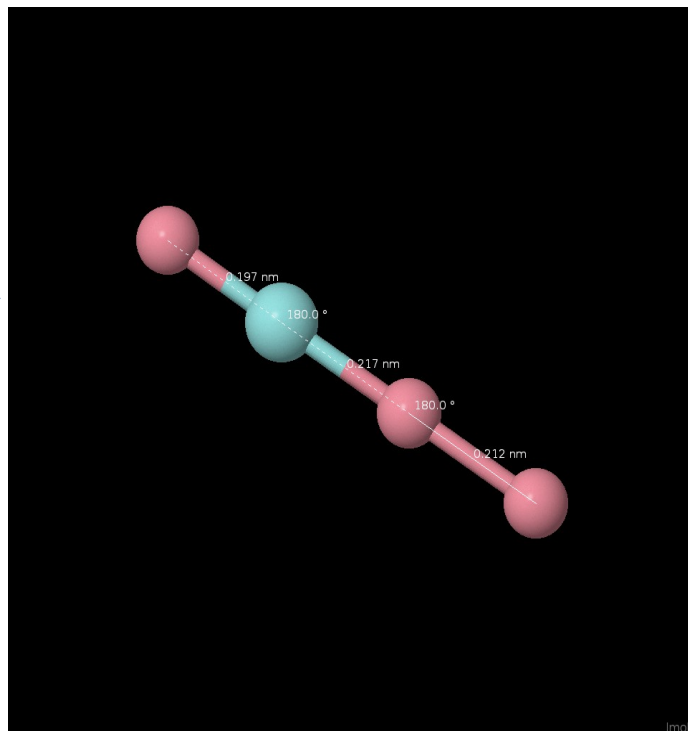
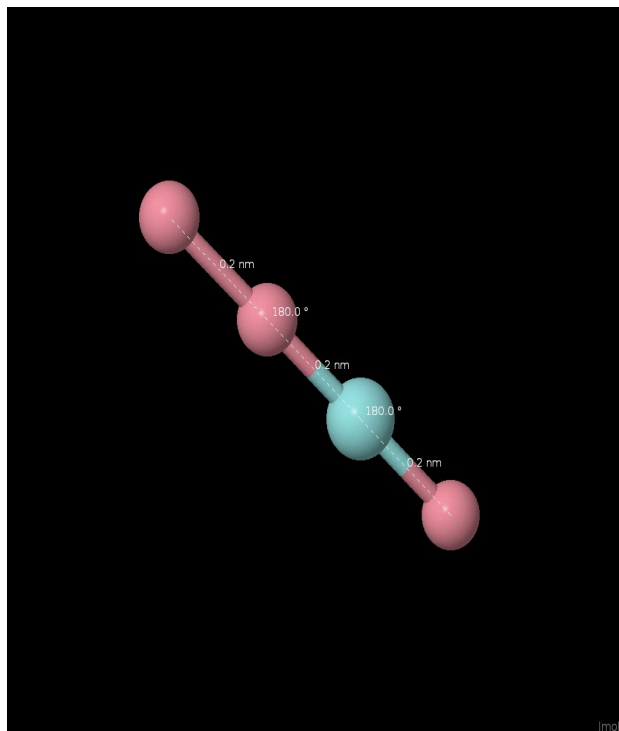
atom	0	0	0	Co
atom	1	0.75	0	Zr
atom	2	2	0	Co
atom	1	2	0	Co



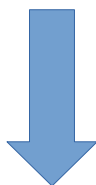
atom	1.47485134	0.10028169	-0.00000000	Zr
atom	2.60957692	2.53365794	-0.00000000	Co
atom	0.51857539	2.11589245	0.00000000	Co

Energy = -212992.883632 eV

## Structure-3



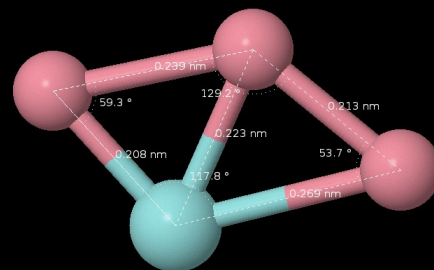
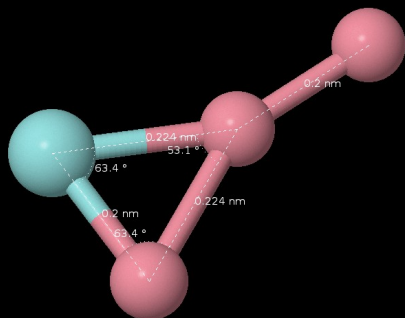
atom	0	0	0	Co
atom	0	0	2	Co
atom	0	0	4	Zr
atom	0	0	6	Co



atom	0.00000001	0.00000006	-0.16985270	Co
atom	-0.00000000	-0.00000008	1.95214133	Co
atom	-0.00000002	-0.00000002	4.12362648	Zr
atom	0.00000001	0.00000004	6.09408489	Co

Energy = -212990.966254 eV

## Structure-4



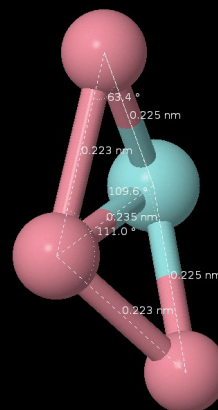
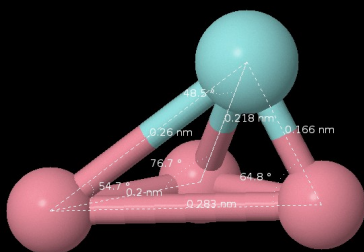
atom	-1	0	0	Co
atom	1	0	0	Zr
atom	0	2	0	Co
atom	0	4	0	Co



atom	-0.74633737	-0.35020863	-0.00003932	Co
atom	0.97285898	0.82114447	0.00002960	Zr
atom	-0.89543623	2.03991114	0.00004292	Co
atom	0.66891462	3.48915302	-0.00003321	Co

Energy = -212992.883826 eV

## Structure-5



atom	0	0	0	Co
atom	0	0	2	Co
atom	0	2	2	Co
atom	1.5	1.5	1.5	Zr



atom	0.43493234	-0.26015163	-0.08954909	Co
atom	-0.27884462	0.08996056	1.99363172	Co
atom	-0.04521879	2.23124079	2.56730070	Co
atom	1.38913107	1.43895028	1.02861668	Zr

Energy = **212992.878588 eV**