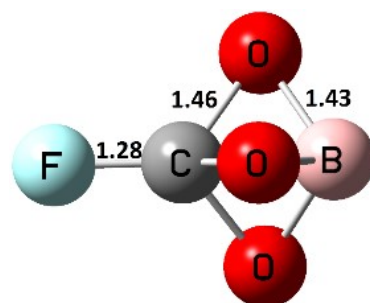
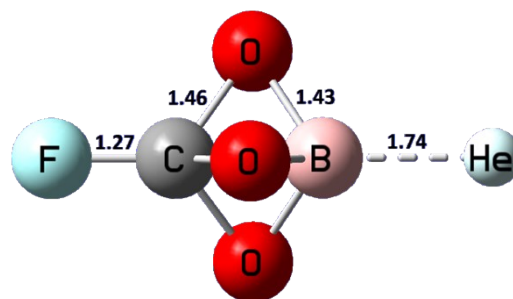




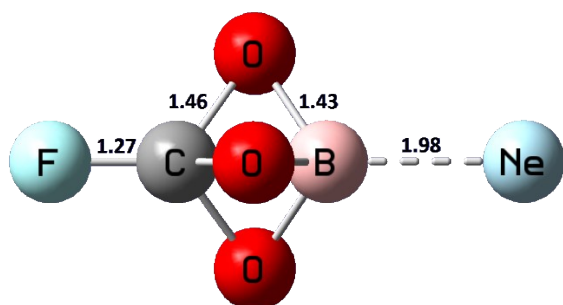
ωB97X-D/def2-TZVP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.000000	0.000000	-1.169522
2	6	0	0.000000	0.000000	0.335875
3	9	0	0.000000	0.000000	1.619472
4	8	0	0.000000	1.242926	-0.447621
5	8	0	-1.076405	-0.621463	-0.447621
6	8	0	1.076405	-0.621463	-0.447621



ωB97X-D/def2-TZVP

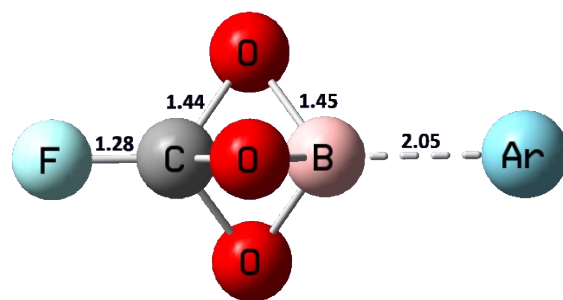
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.057650	-0.000980	0.001261
2	6	0	-0.459602	0.000102	-0.000097
3	9	0	-1.744895	0.001388	-0.001696
4	8	0	0.322605	1.234675	-0.086995
5	8	0	0.321518	-0.693863	-1.025130
6	8	0	0.318590	-0.542172	1.113825
7	2	0	2.735853	0.001338	-0.002028



CBFO₃Ne

ω B97X-D/def2-TZVP

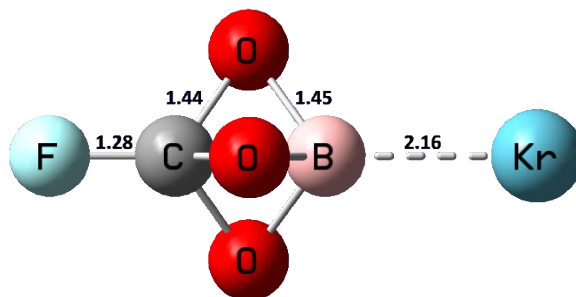
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.577535	-0.002284	0.002313
2	6	0	-0.934632	-0.000283	-0.000484
3	9	0	-2.219614	0.003778	-0.002889
4	8	0	-0.156792	-0.172996	1.228889
5	8	0	-0.149312	1.148301	-0.464193
6	8	0	-0.154419	-0.979126	-0.761539
7	10	0	2.638082	0.000969	-0.000792



CBFO₃Ar

ω B97X-D/def2-TZVP

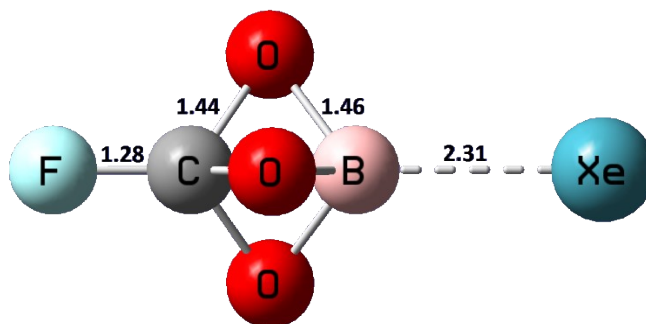
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.275011	0.000733	-0.000188
2	6	0	1.264409	-0.001105	0.000360
3	9	0	2.556526	0.001277	-0.001251
4	8	0	0.502686	-0.486889	1.134190
5	8	0	0.500713	-0.739271	-0.987685
6	8	0	0.499110	1.225439	-0.145205
7	18	0	-2.291122	-0.000153	-0.000020



CBFO₃Kr

ω B97X-D/def2-TZVP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.298304	0.002083	-0.003660
2	6	0	1.841074	-0.000778	0.001799
3	9	0	3.135671	-0.001258	0.001445
4	8	0	1.081903	-0.995644	-0.729010
5	8	0	1.082800	1.129537	-0.499322
6	8	0	1.082221	-0.132039	1.225568
7	36	0	-1.853733	-0.000257	0.000462



CBFO₃Xe

ω B97X-D/def2-TZVP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.729199	0.002380	-0.013508
2	6	0	2.278426	-0.001002	0.005797
3	9	0	3.574811	-0.001321	0.007659
4	8	0	1.526752	1.104550	-0.555495
5	8	0	1.520809	-0.073192	1.227694
6	8	0	1.526161	-1.029407	-0.683371
7	54	0	-1.594067	-0.000178	0.000985