Christopher Hunt
CH 201
Lab 9

Lab 9: Molecular Modeling

Results:

Results begin on the next page.
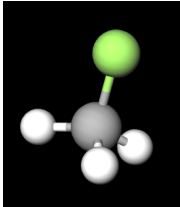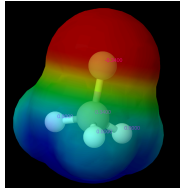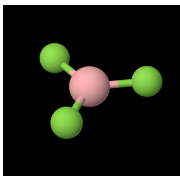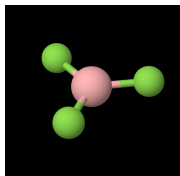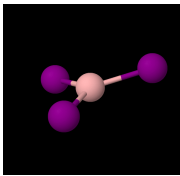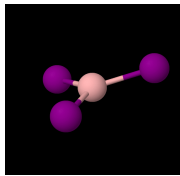
Results Table 1.
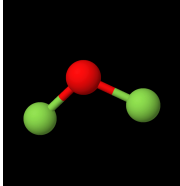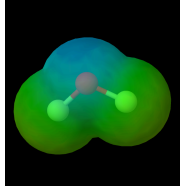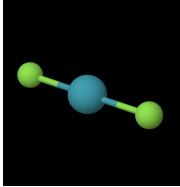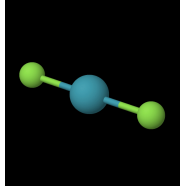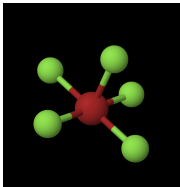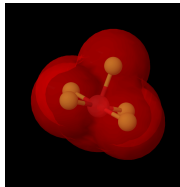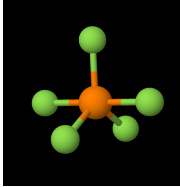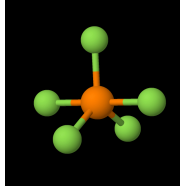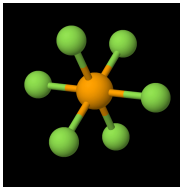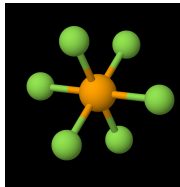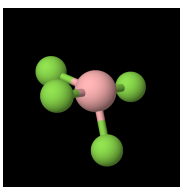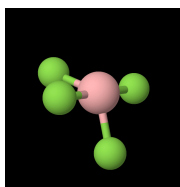
Results Table 1

Formula	Lewis Structure	EG	MG
CH_3F	:F: H–C–H H	Tetrahedral	Tetrahedral
BF_3	:F — B — F: :F:	Trigonal Planar	Trigonal Planar
BI_3	:I — B — I: :I:	Trigonal Planar	Trigonal Planar
OF_2	:F — O — F:	Trigonal Planar	Bent
XeF_2	:F — Xe — F:	Linear	Linear
BrF_5	:F: :F – ¦ ⁄ F: :F ⁄ Br ⸱ F:	Trigonal Bipyramidal	Trigonal Bipyramidal
PF_5	:F: :F – P – F: :F ⸱ F:	Trigonal Bipyramidal	Trigonal Bipyramidal
SeF_6	:F: :F: :F – Se – F: :F: :F:	Octahedral	Octahedral
BF_4^-	[:F: :F:]⁻ B :F: :F:	$\frac{FC}{B}: 3-4=-1$ Tetrahedral	Bent
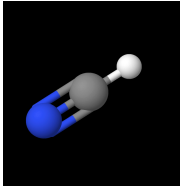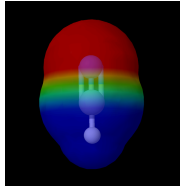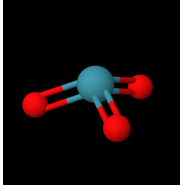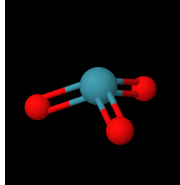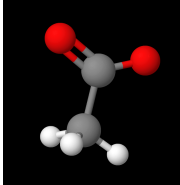
Results Table 1

Formula	Lewis Structure	EG	MG
HCN	H — C ≡ N:	Linear	Linear
XeO_3	$\ddot{O} = \overset{\cdot\cdot}{X}e = \ddot{O}$ with $\overset{\|}{:O:}$ below	Trigonal planar	Bent
$C_2H_3O_2^-$	$[H-\overset{H}{\underset{H}{C}} - \overset{:O:}{C} - \ddot{O}:]^-$	Octahedral	Octahedral

Results Table 2.

Formula	MolView	Bond Length (nm)	Bond Angles (degree)	MEP	Polarity
CH_3F		C-H: 0.109 C-H: 0.109 C-H: 0.109 C-F: 0.136	F-C-H: 108.8 F-C-H: 108.8 H-C-H: 110.2 H-C-H: 110.2 Average: 109.5		δ+ Polar δ-
BF_3		B-F: 0.137 B-F: 0.137 B-F: 0.137	F-B-F: 120 F-B-F: 120 F-B-F: 120 Average: 120		Nonpolar
BI_3		B-I: 0.212 B-I: 0.212 B-I: 0.212	I-B-I : 120 I-B-I: 120 I-B-I: 120 Average: 120		Nonpolar

OF_2		O-F: 0.141 O-F: 0.141	F-O-F: 110.4 Average: 110.4		δ+ Polar δ-
XeF_2		Xe-F: 0.2 Xe-F: 0.2	F-Xe-F: 180 Average: 180		Nonpolar
BrF_5		Br-F: 0.171 Br-F: 0.171 Br-F: 0.171 Br-F: 0.171 Br-F: 0.171	F-Br-F: 90 F-Br-F: 90 F-Br-F: 90 F-Br-F: 90 F-Br-F: 90 Average: 90		δ+ Polar δ+
PF_5		P-F: 0.167 P-F: 0.167 P-F: 0.167 P-F: 0.167 P-F: 0.167	F-P-F: 120 F-P-F: 120 F-P-F: 120 F-P-F: 90 F-P-F: 90 F-P-F: 90 Average: 105		Nonpolar
SeF_6		Se-F: 0.176 Se-F: 0.176 Se-F: 0.176 Se-F: 0.176 Se-F: 0.176 Se-F: 0.176	F-Se-F: 90 F-Se-F: 90 F-Se-F: 90 F-Se-F: 90 F-Se-F: 90 F-Se-F: 90 Average: 90		Nonpolar
BF_4		B-F: 0.137 B-F: 0.137 B-F: 0.137 B-F: 0.137	F-B-F: 120 F-B-F: 120 F-B-F: 90 F-B-F: 90 Average: 105		Nonpolar

HCN		H-C: 0.107 N-C: 0.116	H-C-N: 180 Average: 180		δ+ Polar δ-
XeO_3		Xe-O: 0.2 Xe-O: 0.2 Xe-O: 0.2	O-Xe-O: 109.5 O-Xe-O: 109.5 O-Xe-O: 109.5 Average: 109.5		Nonpolar
$C_2H_3O_2$		C-O: 0.126 C-O: 0.126 C-C: 0.152 C-H: 0.109 C-H: 0.109 C-H: 0.109	H-C-H: 108.4 H-C-H: 108.4 H-C-H: 108.4 H-C-C: 111.4 H-C-C: 111.4 H-C-C: 111.4 O-C-O: 129.9 O-C-C: 115.3 O-C-C: 115.3 Average: 113.3		δ+ Polar δ+

Discussion and Conclusion:

The purpose of this lab was to expand on the Lewis Model with the VSEPR molecular model theory. This was done by first drawing the Lewis structure and then modeling the same molecules with MolView. The VSEPR theory explains how the arrangement of atoms and lone pairs of electrons in a molecule affects its shape. The theory states that electrons repel each other and will position themselves as far apart as possible, resulting in different molecular geometries. One example of a real-world application of the VSEPR model is in the field of drug development, where the knowledge of the molecular shape of a drug molecule is important in determining its interactions with biological receptors. Using MolView we are able to visualize the polarity of molecules which helped broaden our understanding of how the distribution of electrons and the polarity affects its shape.