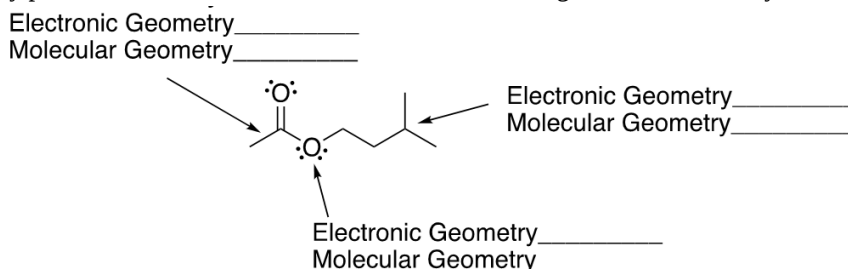


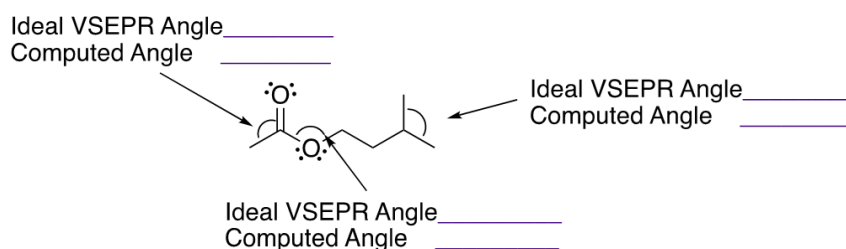
1.4: Exercise Questions

1. Consider the structure of the following isoamyl acetate molecule. This molecule is partially responsible for the taste and smell of a banana.

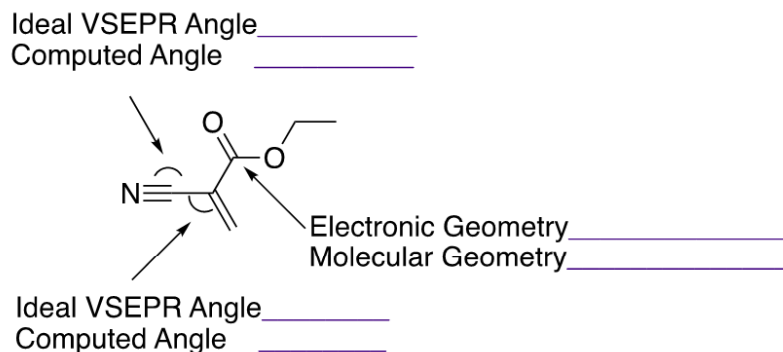
A. Using VSEPR theory please show the indicated electronic and molecular geometries of isoamyl acetate.



B. Draw isoamyl acetate in Avogadro and optimize its geometry. Measure the indicated bond angles and compare them to their predicted ideal bond angles.

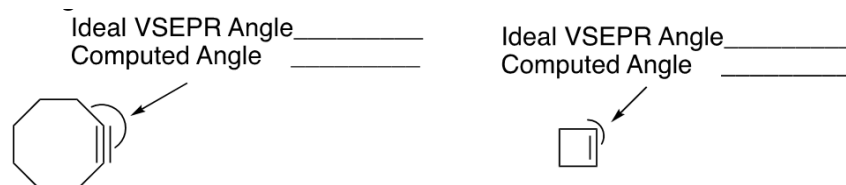


2. Please draw and optimize ethyl cyanoacrylate, as shown below, using Avogadro. Please use the bond angles in this structure and your knowledge of VSEPR to provide the missing information. Ethyl cyanoacrylate is often used as a component of fast drying glues often referred to as superglue.



3. Not all molecules have bond angles or molecular geometries that match what is predicted via VSEPR. There are instances when VSEPR theory breaks down and you have deviations in bond angles and molecular geometry.

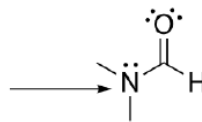
A. One instance of VSEPR theory failing to accurately predict the geometry of an atom occurs when a ring constrains the preferred bond angle. Please draw both cyclooctyne and cyclobutene and optimize their structure in Avogadro to provide the missing information.



B. Another instance when VSEPR theory fails to accurately predict the geometry of an atom is when an atom containing a non-bonding pair of electrons is adjacent to a double bond, which results in partial double bond character. For example, N,N-dimethylformamide (DMF) has a nitrogen with a non-bonding pair of electrons next to a carbonyl functional group. In this

case the nitrogen-carbonyl carbon bond will have the bond strength and length in between a single and double bond. This behavior is known as electron delocalization, and we will learn more about it in subsequent exercises. Please draw and optimize the geometry of a molecule of DMF in Avogadro and provide the missing information.

Predicted Molecular Geometry
by VSEPR _____
Computed Molecular Geometry
using Avogadro _____



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