Vibrational spectroscopy, AKA Infrared (IR) Spectroscopy, is a highly useful and beneficial tool for determining structures and functional groups contained in compounds. Although used for many different structure types of polyatomic molecules, this particular Module is dedicated to triatomic molecules with bent and linear spacial molecular geometry.

Introduction

Triatomic molecules are molecules that contain three atoms. The atoms in triatomic molecules can all be the same, as in I$_3$·, all be different, as in HCN, or can be a mix like CO$_2$. Examples include H$_2$O, which is a bent and has a bond angle of 109°, and a linear triatomic molecule such as CO$_2$. All bent tri-atomic molecules belong to the point group C$_{2v}$, while all the liner tri-atomic molecules with an inversion center belong to the D$_{\infty h}$ point group; Those without an inversion center belong to the point group C$_{\infty v}$. This gives these two structures very different infrared spectrum even though they have the same number of atoms.

Linear molecules

Using VESPR theory there are several ways to achieve a linear structure. Tri-atomic molecules where the central atom is using ALL of its electrons in the bonds with the surrounding molecules, or in other words the central atom does not have any lone pairs surrounding it, will give rise to a linear molecule. Examples include \(\text{CO}_2\) and \(\text{BeH}_3\). This electronic configuration gives the central atom a sp hybridization. Triatomic molecules where the central atom does not use all of its electron pairs in the bonds between the other two atoms will, under certain circumstances, also give rise to a linear species. When the central atom is surrounded by three, or four lone pairs in addition to the two elements already attached will also give rise to a linear molecule. Examples include \(\text{KrF}_2\).

Bent Molecules

There are also several ways to give rise to bent molecules using VESPR theory. A tri-atomic molecule with one, or two lone pair on the central atom will also give rise to bent species. One lone pair examples include SO$_2$, and two lone pair examples include H$_2$O

References


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