

## Section 4: Observation 2: Molecules with Double or Triple Bonds

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In each of the molecules considered up to this point, the electron pairs are either in single bonds or in lone pairs. In current form, the Electron Domain model does not account for the observed geometry of  $C_2H_4$ , in which each H-C-H bond angle is  $116.6^\circ$  and each H-C-C bond angle is  $121.7^\circ$  and all six atoms lie in the same plane. Each carbon atom in this molecule is surrounded by four pairs of electrons, all of which are involved in bonding, i.e. there are no lone pairs. However, the arrangement of these electron pairs, and thus the bonded atoms, about each carbon is not even approximately tetrahedral. Rather, the H-C-H and H-C-C bond angles are much closer to  $120^\circ$ , the angle which would be expected if three electron pairs were separated in the optimal arrangement, as just discussed for  $BCl_3$ .

This observed geometry can be understood by re-examining the Lewis structure. Recall that, although there are four electron pairs about each carbon atom, two of these pairs form a double bond between the carbon atoms. It is tempting to assume that these four electron pairs are forced apart to form a tetrahedron as in previous molecules. However, if this were this case, the two pairs involved in the double bond would be separated by an angle of  $109.5^\circ$  which would make it impossible for both pairs to be localized between the carbon atoms. To preserve the double bond, we must assume that the two electron pairs in the double bond remain in the same vicinity. Given this assumption, separating the three independent groups of electron pairs about a carbon atom produces an expectation that all three pairs should lie in the same plane as the carbon atom, separated by  $120^\circ$  angles. This agrees very closely with the observed bond angles. We conclude that the our model can be extended to understanding the geometries of molecules with double (or triple) bonds by treating the multiple bond as two electron pairs confined to a single domain. It is for this reason that we refer to the model as Electron Domain theory.

Applied in this form, Electron Domain theory can help us understand the linear geometry of  $CO_2$

. Again, there are four electron pairs in the valence shell of the carbon atom, but these are grouped into only two domains of two electron pairs each, corresponding to the two  $C=O$  double bonds. Minimizing the repulsion between these two domains forces the oxygen atoms to directly opposite sides of the carbon, producing a linear molecule. Similar reasoning using Electron Domain theory as applied to triple bonds correctly predicts that acetylene,  $HCCH$ , is a linear molecule. If the electron pairs in the triple bond are treated as a single domain, then each carbon atom has only two domains each. Forcing these domains to opposite sides from one another accurately predicts  $180^\circ$  H-C-C bond angles.

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