



Postulates and History of Valence Band Theory (VBT)

Mazumdar Gupta*

Department of Chemistry, University of Uppsala, Uppsala, Sweden

DESCRIPTION

According to the Valence Bond Theory (VBT), all bonds are established between two atoms by the donation of an electron from each atom. This is an incorrect assumption because many atoms connect with delocalized electrons. The VB hypothesis predicts that there are no unpaired electrons in molecular oxygen. The VB theory performs a decent job of explaining the geometries of covalent compounds qualitatively. While the Molecular Orbital (MO) theory is useful for learning about bonding in general, it is more difficult to understand, but it better predicts actual molecular properties than VB theory. Because of discrepancies in the energy levels of orbitals in the molecule, the MO theory predicts electron transitions. MO theory has proven to be more accurate in multiple situations, as a result. The theory of Valence Bonds covers the creation of covalent bonds as well as the electronic structure of molecules. The hypothesis assumes that electrons occupy the atomic orbitals of individual atoms inside a molecule and that electrons from one atom are drawn to the nucleus of another. As the atoms get closer to one another, the attraction grows stronger until the electron density causes repulsion between them. The lowest potential energy is achieved at the minimum distance between the two atoms, and this electron density can be considered what keeps the two atoms together in a chemical bond [1].

Lewis structures are used in valence bond theory. G.N. Lewis proposed these structures in 1916, based on the assumption that chemical bonds are produced by two shared bonding electrons. The Heitler-London theory of 1927 used quantum mechanics to characterize bonding qualities. Schrodinger's wave equation is used to merge the wave functions of two hydrogen atoms. This theory details chemical bond formation between hydrogen atoms in the H₂ molecule. Linus Pauling proposed the valence bond theory in 1928, combining Lewis' pair bonding notion with the Heitler-London theory. The valence bond theory was devised to explain resonance and orbital hybridization. In 1931, Pauling released "On the Nature of the Chemical Bond," a treatise on valence bond theory. The initial computer programmers employed molecular orbital theory to represent chemical

bonding, but since the 1980s, valence bond theory principles have been programmable. In terms of properly explaining real behavior, today's versions of these ideas compete with one another [2].

The covalent bond is formed by the overlapping of two half-filled valence orbitals of two distinct atoms. The electron density between two linked atoms increases due to the overlapping. The molecule now has the property of stability. More than one bond can be created if the atomic orbitals contain more than one unpaired electron, and electrons paired in the valence shell cannot participate in such a bond formation. A covalent bond has a specific direction. There are two types of covalent bonds based on the overlapping pattern: Sigma bonds and pi bonds. The pi bond is created by overlapping atomic orbitals sideways, whereas the sigma bond is formed by overlapping atomic orbitals along the inter-nucleus axis [3]. The creation of covalent bonds in many molecules can be explained by the maximum overlap requirement stated by the valence bond theory. One of its most essential applications is this. For example, the variation in the length and strength of chemical bonds in H₂ and F₂ molecules can be explained by differences in their overlapping orbitals. The overlap of the 1s orbital of the hydrogen atom and the 2p orbital of the fluorine atom forms the covalent bond in an HF molecule, as explained by the valence bond theory [4]. The valence bond theory has several flaws, including a failure to explain carbon's tetravalency, no insight into electron energies, the theory assumes that electrons are localized in specific areas, no quantitative interpretation of the thermodynamic or kinetic stabilities of coordination compounds, no distinction between weak and strong ligands, and no explanation for coordination compounds' colour [5].

The formation of covalent bonds can typically be explained using the valence bond theory. One example is the diatomic fluorine molecule F₂. Single covalent bonds develop between fluorine atoms. The F-F bond is formed by overlapping Pz orbitals, each of which has one unpaired electron. In hydrogen H₂, a similar situation occurs, but the bond lengths and strength between H₂ and F₂ molecules are different. Hydrogen and fluorine create a covalent link in Hydrofluoric Acid (HF). The

Correspondence to: Mazumdar Gupta, Department of Chemistry, University of Uppsala, Uppsala, Sweden, Email: Gupta@gmail.com

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overlap of the hydrogen 1s orbital and the fluorine 2Pz orbital, both of which have an unpaired electron, generates this link. These electrons are shared in a covalent link between the hydrogen and fluorine atoms in HF.

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