

## Editorial Note on Chemical Bonding of Water

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### DESCRIPTION

Water ( $H_2O$ ) is a simple triatomic bent molecule with  $C_{2v}$  molecular symmetry and a  $104.5^\circ$  bond angle between the center oxygen and hydrogen atoms. Even though it is one of the simplest triatomic compounds, its chemical bonding scheme is complicated since several of its bonding parameters, Instead, several traditional and advanced bonding models are discussed below, including the simple Lewis and VSEPR structure, valence bond theory, molecular orbital theory, isovalent hybridization, and Bent's rule, to provide a comprehensive bonding model for  $H_2O$ , explaining and rationalizing the various electronic and physical properties and features manifested by its peculiar bonding arrangements.

The central oxygen atom and the two peripheral hydrogen atoms form two sigma bonds, with oxygen having two lone pairs of electrons, according to the Lewis structure of  $H_2O$ . According to valence bond theory,  $H_2O$  is  $sp^3$  hybridized, meaning the  $2s$  atomic orbital and the three  $2p$  orbitals of oxygen are hybridized to generate four new hybridized orbitals that overlap with the hydrogen  $1s$  orbitals and engage in bonding. As a result, the shape and bond angle of  $sp^3$  hybridization are anticipated to be tetrahedral and  $109.5^\circ$ , respectively. This agrees with the true binding angle of  $104.45$  degrees.

The electron repulsion of the two lone pairs occupying two  $sp^3$  hybridized orbitals is generally used to explain the disparity between the expected and measured bond angles. The geometry and bond angle of H can be predicted using valence bond theory. The electronic states predicted by  $2O$  do not match the empirically measured reality. The two sigma bonds, as well as the two lone pairs, have the same energy in the valence bond model since they are both in the same bonding and nonbonding orbitals, corresponding to two energy levels in the photo electronic spectrum.

Advanced or second order atomic orbital mixing that does not create simple  $sp$ ,  $sp^2$ , or  $sp^3$  hybridization schemes is referred to as isovalent hybridization. Because varying fractions of  $s$  and  $p$  orbitals are blended to ensure optimal bonding, bonding orbitals for molecules with lone pairs are isovalent hybrids. Isovalent hybridization is used to explain bond angles that are incompatible with the generalized simple  $sp$ ,  $sp^2$ , and  $sp^3$  hybridization. True hybridization of molecules containing lone pairs is determined by the amount of  $s$  and  $p$  characters in the central atom, which is connected to its electronegativity.

Since the early to mid-1900s, the controversy between Molecular Orbital Theory and Valence Bond Theory has raged. Despite the on-going disagreement over which model best depicts the genuine bonding pattern of molecules, scientists currently regard the MO and VB theories as complementary and compatible. Both MO and VB theories are frequently employed nowadays, but for typically different objectives, thanks to the advent of current high-speed computers and powerful molecular modeling tools. In general, MO theory can predict the system's ground state energy, distinct electronic states energies of bonding and nonbonding orbitals, and magnetic and ionization properties with great accuracy. VB theory, on the other hand, has long been used to predict bond angle and mechanism drawing.

Although the procedure is more sophisticated, modern valence bond theory can supply the same electronic information as MO theory. Furthermore, contemporary VB theory can forecast excited state energies in a way that MO theory cannot. The truth is that both theories are equally crucial in understanding chemical bonding, and while none is totally comprehensive, the two together create a comprehensive picture of chemical bonds.

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