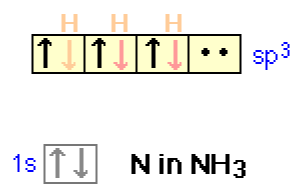
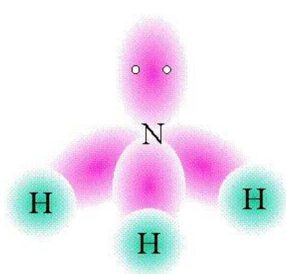
LONE PAIR ELECTRONS IN HYBRID ORBITALS

If lone pair electrons are present on the central atom, these can occupy one or more of the sp3 orbitals. This causes the molecular geometry to be different from the coordination geometry, which remains tetrahedral.

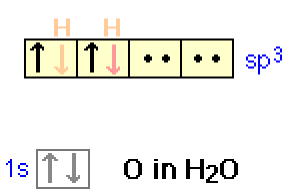


In the **ammonia** molecule, for example, the nitrogen atom normally has three unpaired p electrons, but by mixing the 2s and 2p orbitals, we can create four sp3-hybrid orbitals just as in carbon. Three of these can form shared-electron bonds with hydrogen, resulting in ammonia, NH3. The fourth of the sp3 hybrid orbitals contains the two remaining outer-shell electrons of nitrogen which form a non-bonding lone pair. In acidic solutions these can coordinate with a hydrogen ion, forming the ammonium ion NH4+.



sp^3 hybrid orbitals (tetrahedral)

Although no bonds are formed by the lone pair in NH3, these electrons do give rise to a charge cloud that takes up space just like any other orbital.



In the **water** molecule, the oxygen atom can form four sp3 orbitals.

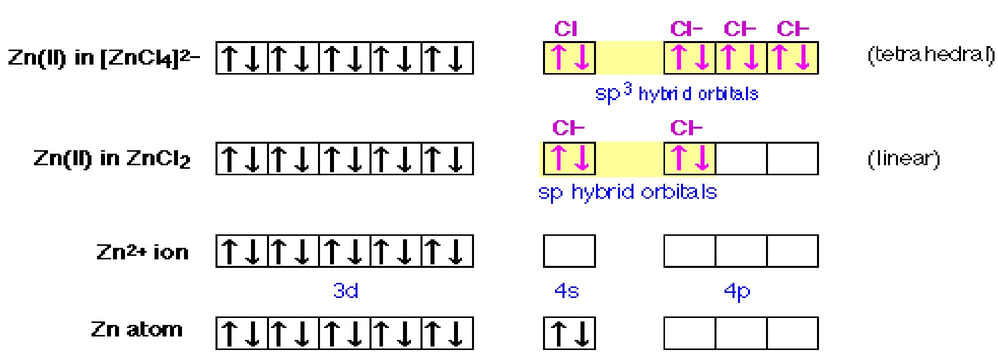
Two of these are occupied by the two lone pairs on the oxygen atom, while the other two are used for bonding.

The observed H-O-H bond angle in water (104.5°) is less than the tetrahedral angle (109.5°); one explanation for this is that the non-bonding electrons tend to remain closer to the central atom and thus exert greater repulsion on the other orbitals, thus pushing the two bonding orbitals closer together.

Molecular ions

Hybridization can also help explain the existence and structure of many **inorganic molecular ions.** Consider, for example, electron configurations of **zinc** in the compounds in the illustrations below.

The **tetrachlorozinc ion** (top row) is another structure derived from zinc and chlorine. As we might expect, this ion is tetrahedral; there are four chloride ions surrounding the central zinc ion. The zinc ion has a charge of +2, and each chloride ion is –1, so the net charge of the complex ion is –2.



At the bottom is shown the electron configuration of atomic zinc, and just above it, of the divalent zinc ion. Notice that this ion has no electrons at all in its 4-shell. In zinc chloride, shown in the next row up, there are two equivalent chlorine atoms bonded to the zinc. The bonding orbitals are of sp character; that is, they are hybrids of the 4s and one 4p orbital of the zinc atom. Since these orbitals are empty in the isolated zinc ion, the bonding electrons themselves are all contributed by the chlorine atoms, or rather, the chloride ions, for it is these that are the bonded species here. Each chloride ion possesses a complete octet of electrons, and two of these electrons occupy each sp bond orbital in the zinc chloride complex ion. This is an example of a **coordinate covalent bond**, in which the bonded atom contributes both of the electrons that make up the shared pair.

Source: http://www.chem1.com/acad/webtext/chembond/cb06.html