

*Chemistry 2000: MO and VB descriptions of  
bonding*

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## *MO descriptions of bonding*

To describe the bonding in a molecule using **MO theory**, proceed as follows:

- ▶ Look at the valence AOs and, if available, at the AO energies.
- ▶ Separate the AOs into sigma-type and pi-type.
- ▶ Number of sigma MOs = number of sigma-type AOs
- ▶ Number of pi MOs = number of pi-type AOs
- ▶ Based on AO energies, say which AOs will combine with which to make MOs.
- ▶ Identify any (exactly or approximately) nonbonding MOs obtained from the AOs.
- ▶ Draw a reasonable MO diagram.
- ▶ Populate it with the valence electrons.
- ▶ Compute the bond order or answer any questions asked about the molecule.

## *VB descriptions of bonding*

To describe the bonding in a molecule using **VB theory**, proceed as follows:

- ▶ Start by determining the electronic geometry at each non-terminal atom using VSEPR theory.
- ▶ Use the following table:

Electronic geometry	Hybridization	Left-over p orbitals
Linear	sp	2
Trigonal planar	sp <sup>2</sup>	1
Tetrahedral	sp <sup>3</sup>	0

- ▶ For the terminal atoms, you can also determine hybridization **or** (my preference) use an unhybridized unfilled valence orbital.
- ▶ Identify any orbitals which will contain lone pairs.
- ▶ Start with the sigma bonds. Describe each of these as being made by combining the appropriate AOs (hybridized or not).
- ▶ Describe any pi bonds as being made by combining “left-over” p orbitals.