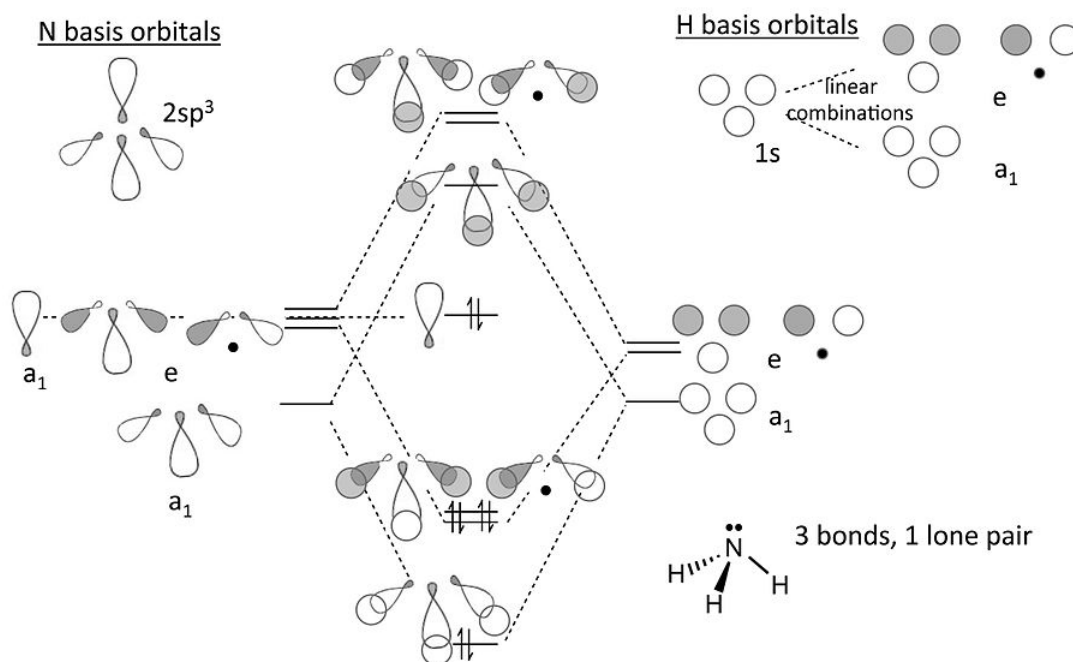


2.9: Building up the MOs of More Complex Molecules- NH_3 , P_4

MO diagram for NH_3

We can now attempt the MO diagram for NH_3 , building on the result we obtained with triangular H_3^+ .

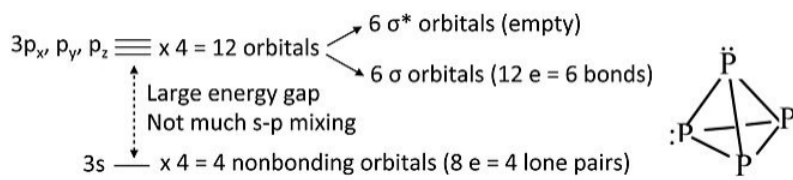


Notes on the MO diagram for ammonia:

- Viewed end-on, a p-orbital or an sp_x hybrid orbital looks just like an s-orbital. Hence we can use the solutions we developed with s-orbitals (for H_3^+) to set up the σ bonding and antibonding combinations of nitrogen sp^3 orbitals with the H 1s orbitals.
- We now construct the sp^3 hybrid orbitals of the nitrogen atom and orient them so that one is “up” and the other three form the triangular base of the tetrahedron. The latter three, by analogy to the H_3^+ ion, transform as one totally symmetric orbital (“ a_1 ”) and an e-symmetry pair. The hybrid orbital at the top of the tetrahedron also has a_1 symmetry.
- The three hydrogen 1s orbitals also make one a_1 and one (doubly degenerate) e combination. We make bonding and antibonding combinations with the nitrogen orbitals of the same symmetry. The remaining a_1 orbital on N is non-bonding. The dotted lines show the correlation between the basis orbitals of a_1 and e symmetry and the molecular orbitals
- The result in the 8-electron NH_3 molecule is **three N-H bonds** and **one lone pair** localized on N, the **same as the valence bond picture** (but much more work!).

P_4 molecule and P_4^{2+} ion:

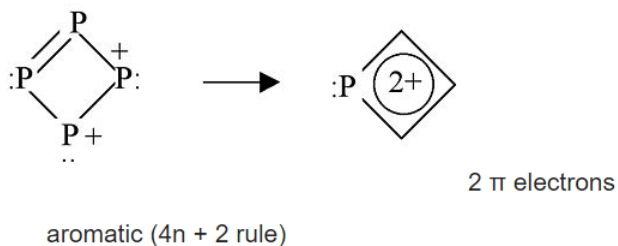
By analogy to NH_3 we can construct the MO picture for one vertex of the P_4 tetrahedron, and then multiply the result by 4 to get the bonding picture for the molecule. An important difference is that there is relatively little s-p hybridization in P_4 , so the lone pair orbitals have more s-character and are lower in energy than the bonding orbitals, which are primarily $\text{p}\sigma$.



Take away 2 electrons to make P_4^{2+}

Highest occupied MO is a bonding orbital → *break one bond, 5 bonds left*

Square form relieves ring strain, ($60^\circ \rightarrow 90^\circ$)



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