Comprehensive MO Review Worksheet: Working through an example, PH2F3.

Work in groups of three or four to complete the following assignment.

1. Let’s get started by drawing a Lewis diagram of PH2F3 and stating its shape according to VSEPR theory. There are three isomers.

2. Next, find the symmetry elements present and determine the point group of each isomer. For the highest order point group, generate a multiplication table and use similarity transforms to determine which are in the same class. Use only this point group for the remaining steps.

3. Now, generate the character table for this point group using transforms on a basis (such as an orbital), 1/-1/0 for symmetric, antisymmetric or no change; as well as the great orthogonality theorem. The table should include symmetries for p-orbitals, d-orbitals, and rotational axes.

4. Now for the fun part. Let’s construct the MO. Start by focusing on the PH2 portion. Find the symmetry of the H atom SALCS and combine these SALCs with the central phosphorous to get an intermediary MO diagram. Don’t worry about exact energies for the MO’s, focus more on reasonable symmetry and energy matching.

5. Now, we need to deal with the F atom portion. Find the symmetries and generate the SALCs of the F atoms. Combine these SALCs with the PH2 you have already generated to get the final MO diagram. Don’t forget about hybridization. Don’t worry about exact energies for the MO’s, focus more on reasonable symmetry and energy matching.

6. Use either intuitive inspection or projection operators to draw pictorial diagrams of each MO.