Workshop 2 Molecular Orbitals and Reactivity

Vinyldimethylamine (1) can react as a base—for example, with hydrochloric acid—in two different ways. In this problem, we will think about these two acid-base reactions from the perspective of molecular orbitals.



- 1. In 1, what is the hybridization state of each atom heavier than hydrogen?
- 2. **1** has a conjugated π system. Given your answer above, how many atoms contribute a *p* orbital to that system? How many electrons do they contribute? (*Note:* These two numbers do not have to be the same.)
- 3. In the space below, draw a molecular orbital diagram for **1**, and fill the orbitals with the appropriate number of electrons.



- 4. Molecule **1** reacts with an acid by donating electrons from the highest-energy occupied molecular orbital. Which orbital is that? Where are the electrons in that orbital?
- 5. What would the two possible protonation products of **1** be? Use "electron pushing" to show how these products would be formed.
- 6. Which product is preferred, and why?