

Additional Problems – MO Theory (Chapter 5)

1. Please re-draw the MO diagrams you obtained for Practice Problems 5.8(a) and 5.10(a). These should show the σ_{2p} and π_{2p} molecular orbitals in different order, energetically. How do we rationalize this difference? Please explain as specifically as possible.

2. Please prepare the first-order MO diagram for ammonia, NH_3 . Show all your work, including:
 - a. Point-group determination
 - b. Determination of SALCs for outer atoms
 - i. basis set
 - ii. reducible representation
 - iii. decomposition into irreducible representations
 - iv. projections – SALC sketches and equations
 - c. Symmetries of interacting orbitals on the central atom
 - d. MO correlation diagram