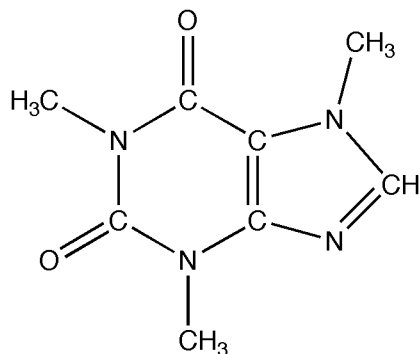


Exercise 1: Hybrid orbitals and molecular orbital theory

1. What is the hybridization of each of the carbon, oxygen, and nitrogen atoms in caffeine (pictured below)?



2. Predict the **bond angle** of each of the atoms in the ring structure of caffeine.

3. Will the atoms in the ring portion of caffeine all lie in the same **plane** (i.e., which would make caffeine a planar molecule)? Explain your reasoning either way.

4. Draw the **molecular orbital** (MO) diagrams for Be_2^+ and Be_2 . Yes, I know they are the same diagram with different numbers of electrons but draw them side by side anyway.

5. Calculate the **bond order** for Be_2^+ and Be_2 . What can you conclude about Be_2 ?