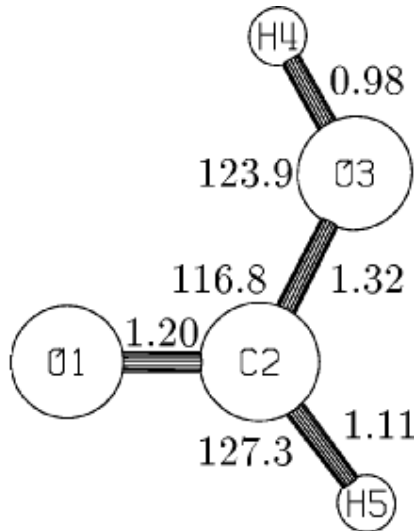
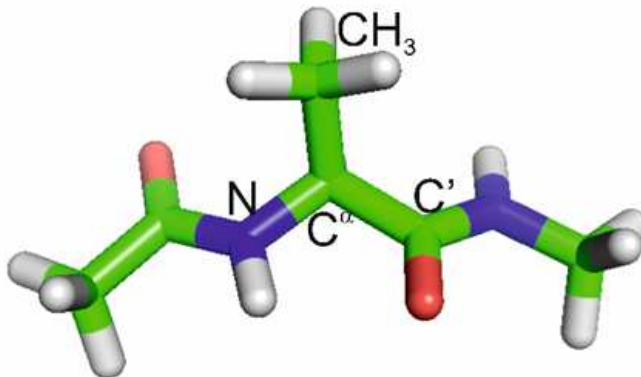


Problem set 1**Due March 7, 2024**

1. Based on the picture of formic acid (HCOOH) in which bond lengths (values in \AA) and bond angles (values in deg) are shown and assuming that the molecule is planar write down the Z-matrix of this molecule.



2. Define the improper dihedral angle that defines the chirality of alanine so that this angle be negative for the terminally-blocked L-alanine molecule shown below. Sketch a picture of D-alanine and demonstrate that the improper-dihedral angle just defined is positive for opposite chirality.



- How many coordinates are necessary to define the energy surface of a system consisting of 2 water molecules (a water dimer) *in vacuo*? Try to define these coordinates.
- In the potential-energy map of glycolamide shown below (Lapinski et al., *J. Phys. Chem. A*, 2019, 123, 3831-3839) mark two energy minima, the saddle point that separates them and draw the approximate reaction path linking these minima.

