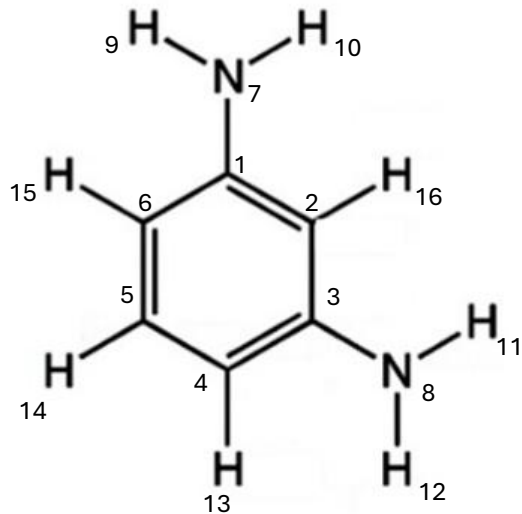
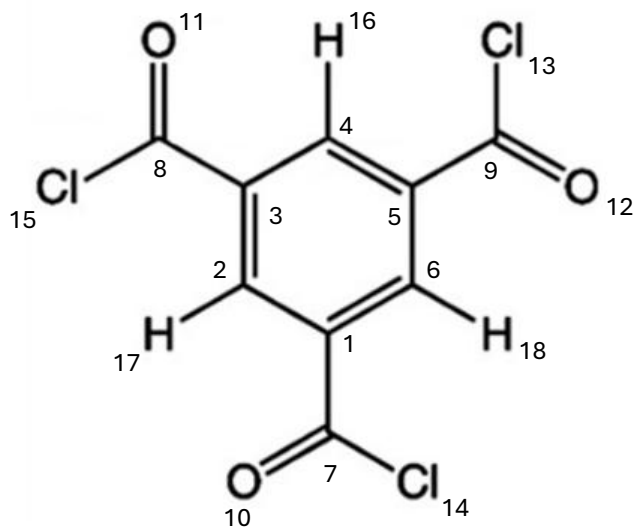


Full molecule according to atom ID for lammps template files:

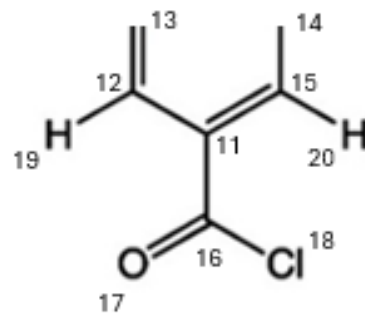
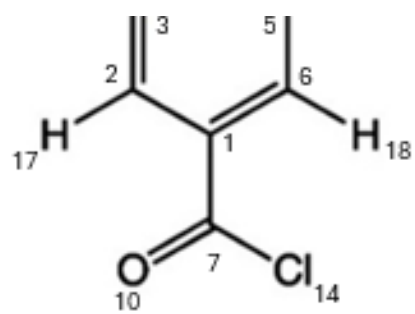
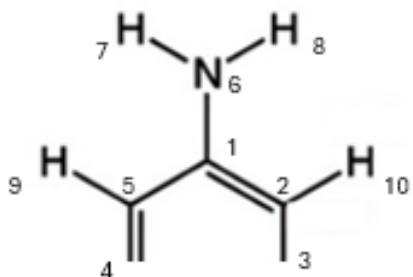
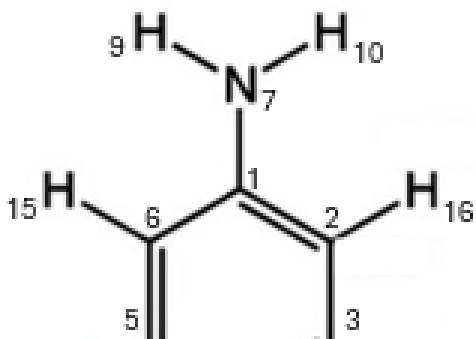


(a) MPD



(b) TMC

Pre molecule generated from individual lammps template file:



Molecule atom typing

