

Fig 1- Ethyle acetate chemical structure

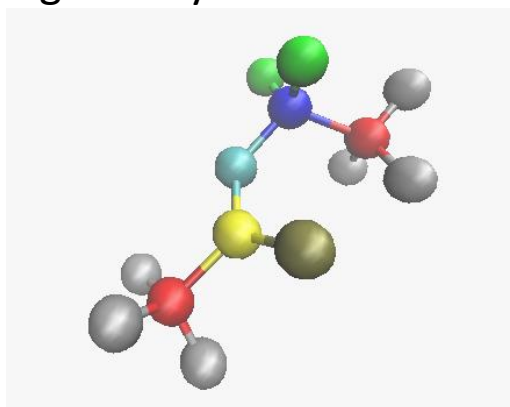


Fig 2- Ethyle acetate produced from moltemplate and plotted using topotool (on VMD)

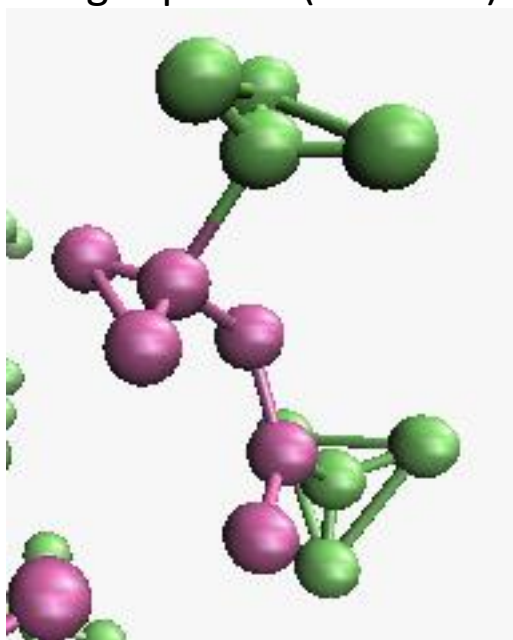


Fig 3- Ethyle acetate from the Lammps-trajectory file using VMD