Computational Chemistry and Materials Modeling
Homework 3 – additional problems

1. Exercise. Using a case study of 3-oxopentanedial (CHO–CH_2–CO–CH_2–CHO) and formaldehyde molecules show that C=O bonds can be identified using vibrational spectroscopy by the corresponding quasilocalized IR-active C-O stretching modes. Explain the observed IR intensities and spectral positions. In the above two molecules replace C=O by C–O–H and explain the difference from the perspective of C-O stretching modes. As another counterexample show a molecule in which C=O bonds loss their "identity" in IR spectrum. Rationalize the obtained results: when a bond can be robustly identified through vibrational spectroscopy?

Also, for 3-oxopentanedial plot IR and Raman spectra and interpret all the prominent peaks.

2. Exercise. Using Web resources, briefly describe significance of vibrational spectroscopy of amide I, II, and III modes.