

## Computational Chemistry and Materials Modeling

### Homework 5, due date is set in Canvas LMS

**1. Lab.** Using a case study of 3-oxopentanedial ( $\text{CHO-CH}_2\text{-CO-CH}_2\text{-CHO}$ ) and formaldehyde molecules show that  $\text{C=O}$  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  $\text{C=O}$  by  $\text{C-O-H}$  and explain the difference from the perspective of C-O stretching modes. As another counterexample show a molecule in which  $\text{C=O}$  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.

**3. Exercise.** No exercise for 2017.

**4. Exercise.** In vibrational spectroscopy of organic molecules, what is typical highest energy vibrational band active in IR spectra? Explain your answer.

**5. Exercise.** Which nuclei of paracetamol molecule produce no strong NMR signal for their most abundant isotope?