

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 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.

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?