JSS27 Where are the protons? Practical work of vibrational spectroscopy, laboratory instructions

6 x 3/4 person-group

Idea: To familiarize FTIR spectra of simple organic compounds. We measure relative concentrations of COOH and COO^- groups from acetic acids at different pH with FTIR spectrometer. Using this information the pKa value of the acetic acid is determined by utilizing Henderson–Hasselbalch equation.

Place: Organic Chemistry Laboratory. Let´s get together in the class-room (YAB310) and walk to the lab group by group.

pH testing (estimated time 20 min):
A set of mixtures of Acetic acid (99.7%) and NaOH (10M) is provided. The pH values ranges from 2 – 10. Test the pH values of the solutions with the pH meter provided.

At the FTIR (estimated time 20 min)
Measure the first background with air.
Water spectrum: Inject a small droplet of H_2O
Measure 2nd background with H2O
Sample spectrum: Inject a sample to the measurement cell and measure a spectrum
Repeat a set with different pHs

Save the data in dpt format and transfer to JYU-Network computer

For the data analysis, identify the COOH bands (1730cm^{-1} / 1257 cm^{-1}) and COO^- bands (1579cm-1 / 1406 cm-1) of acetic acid or its salt.

Then, follow the instructions in
https://docs.google.com/spreadsheets/d/1cURsJGEpok3zN5ctKLlMyogPMGiLxGT_oeJGL-W8OiY/edit?usp=sharing

Time-table:
13:00 - 13:20 Group 1 pH testing
13:20 – 13:40 Group 2 pH testing, Group 1 FTIR
13:40 – 14:00 Group 3 pH testing, Group 2 FTIR
14:00 – 14:20 Group 4 pH testing, Group 3 FTIR
14:20 – 14:40 Group 5 pH testing, Group 4 FTIR
14:40 – 15:00 Group 6 pH testing, Group 5 FTIR
15:00 – 15:20 Group 6 FTIR

The data-analysis can be done in the class-room with own computers or in the computers in the aula of the biology department.
16:00 – 17:00 Final data-discussion

For reference: Wikipedia or similar. For a more advanced level:
http://pubs.acs.org/doi/abs/10.1021/jp036401t?journalCode=jpcafh