Chemistry 416, Dr. Glaser

Applications of IR/Raman Spectra: Hydrogen Bonding.

In order to distinguish between intra- and intermolecular H-bonding, one usually measures the IR spectra at various concentrations. Intramolecular H-bonding should be independent of concentration while intermolecular H-bonding should dependent on concentration. Given below are two spectra taken at different concentrations for cyclohexylcarbinol and for *ortho*-hydroxyacetophenone.

(a) Draw the structures of these molecules

(b) For each, draw structures for inter- and intramolecular H-bonding

(c) Considering the spectra, which type of H-bonding is preferred?

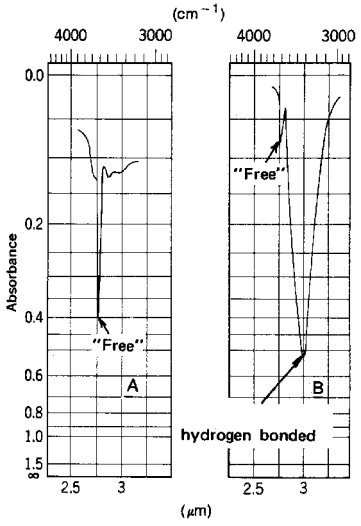

FIGURE 3.17. Infrared spectrum of the O—H stretching region of cyclohexylcarbinol in CCl_4. Peak A at 0.03 *M* (0.406 mm cell); Peak B at 1.00 *M* (0.014 mm cell).

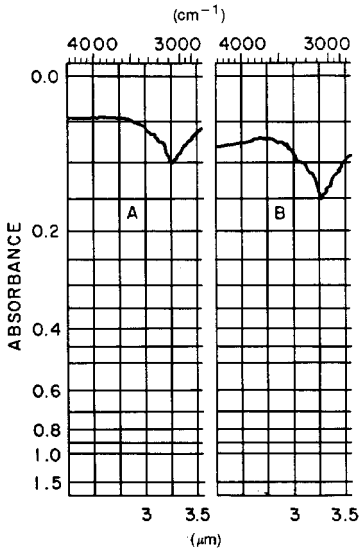

FIGURE 3.18. A portion of the IR spectra of *o*-hydroxyacetophenone. Peak A at 0.03 *M*, cell thickness: 0.41 mm. Peak B at 1.0 *M*, cell thickness: 0.015 mm.

(from Silverstein, page 111)