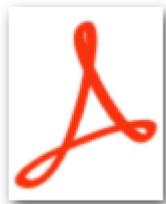# File:Chapter-19 Infrared spectroscopy (Bond Parameter & Hybridization) pp 159-160.pdf

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Chapter-19_Infrared_spectroscopy_(Bond_Parameter_&_Hybridization)_pp_159-160.pdf (0 × 0 pixels, file size: 682 KB, MIME type: application/pdf)

Summary

Description	IR absorption frequency depends on bond properties or bond parameter. Bond strength, masses of the bonded atoms and hybridization state affect the infrared absorption frequency. Bond multiplicity of homonuclei species is directly proportional to the IR absorption frequency. Masses of the bonded atoms are inversely proportional to the IR absorption frequency. Hybridization affects the IR absorption frequency. With increasing power of the hybridization state (PHyb), IR absorption frequency decreases.
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Chapter-19
Infrared spectroscopy
(Bond Parameter & Hybridization)

Arijit Das

IR absorption frequency depends on bond properties or bond parameter. Bond strength, masses of the bonded atoms and hybridization state affect the infrared absorption frequency as follows:

1. Bond multiplicity: Bond multiplicity of homonuclei species is directly proportional to IR absorption frequency (higher frequency or higher wave number cm^{-1}).

i.e. Bond multiplicity of homonuclei species α IR absorption frequency

Eg. C≡C (2150 cm^{-1}) > C=C (1650 cm^{-1}) > C-C (1200 cm^{-1}). Thus Triple bonds (≡) are stronger than double bonds (=) over single (-) bond.

2. Masses of the bonded atoms: Masses of the bonded atoms are inversely proportional to the IR absorption Frequency.

i.e. Masses of the bonded atoms α 1/ IR absorption frequency

Eg. The C-H stretch occurs at about 3000cm^{-1}. As the atom bonded to carbon increases in mass (i.e.atomic weight) then the frequency of vibration decreases (wave numbers cm^{-1} get smaller).

C-H (3000cm^{-1})→C-C (1200cm^{-1})→C-O (1100cm^{-1})→C-Cl (750cm^{-1})→C-Br (600cm^{-1})→C-I (500 cm^{-1})

(At.wt.H -1.008   C – 12.01   O-15.99   Cl-35.45   Br-79.90   I-126.9)

3. Hybridization: Hybridization affects the IR absorption frequency. With increasing power of the hybridization state (P_{Hyb}), IR absorption frequency decreases.

i.e. Power of the hybridization state α 1/ IR absorption Frequency

Eg. Bonds are stronger is in the order   sp (P_{Hyb}=1) > sp^2 (P_{Hyb}= 2) > sp^3 (P_{Hyb}= 3). Thus IR absorption frequency follows the order

≡C-H (P_{Hyb}=1, sp, 3300cm^{-1}) > =C-H (P_{Hyb}= 2, sp^2, 3100cm^{-1}) > -C-H (P_{Hyb}=3, sp^3, 2900cm^{-1})

Related Questions:

Q.1. Arrange the following into their decreasing order of infrared absorption frequency (cm^{-1})

i) CH$_3$-CH$_3$, CH$_2$=CH$_2$, CH≡CH

ii) C-Cl, C-I, C-Br

iii) C-H, C-O, C-C

iv) =C-H, -C-H, ≡C-H

Q.2. Which one of the following will have higher IR absorption frequency (cm^{-1})

    a. C-O   b. C-C   c. C-Cl   d. C-Br

Reference Books:

1. Fourier Transforms in NMR, Optical and Mass Spectroscopy, Alan G. Marshall, Francis R. Verdun, Elsevier, 1990.
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3. Infrared Spectroscopy: Fundamentals and Applications, Barbara H. Stuart, John Wiley & Sons, Ltd, 2004.
4. Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A: Theory and Applications in Inorganic Chemistry, Sixth Edition, Kazuo Nakamoto, John Wiley & Sons, Ltd, 2008.
5. Infrared and Raman spectroscopy principles and spectral interpretation, Peter Larkin, Elsevier, 2011.