Answer on Question #45253, Chemistry, Organic Chemistry

Task: Why assymetric streching for AB2 type molecules have higher frequency than symmetric streching?

Answer:

AB_2 type molecules : The structural information requires that whether such molecules are non-linear or linear. If linear, whether symmetrical (B-A-B) or asymmetrical (B-B-A). The nature of Raman and IR spectra provides sufficient information regarding structural aspects of the molecule.

The presence of PR branch indicates that the molecule is linear. It possesses a centre of symmetry or not, can be decided by rule of mutual exclusion. For example, results of IR and Raman spectra for linear $C0_2$ molecule arc given in the table 5.

Table (5)

Vibration	Raman	IR	Wavenumber cm^{-1}
Symm. Stretch	Active	Inactive	1330
Bending	Inactive	Active (PQR)	667.3
Asymm. Stretch	Inactive	Active (PR)	2349.3

$C0_2$ molecule is linear is indicated by the presence of PR branch in IR spectrum of $C0_2$. It is also evident from the above table that no vibration is simultaneously Raman and IR active. Thus rule of mutual exclusion shows that $C0_2$ molecule has a centre of symmetry.

Nitrous oxide molecule have the following results.

Table (6)

$\bar{\nu}$ cm^{-1}	Infrared	Raman
589	Active (strong, PQR)	—
1285	Active (strong, PR)	Active (strong, polarised)
2224	Active (strong, PR)	Active (strong, depolarised)

The presence of PR branch indicates that N^O molecule is linear. The molecule docs not have a centre of symmetry because at least two of the vibrations arc simultaneously 1R and Raman active. The probable structure is

$$N \equiv N = O$$

The molecule N-N-0 possesses an axis of symmetry along the bond axis. Since PR branches arise due to parallel vibrations, the frequencies at 1285 $cm^{-1}$and 2224 cm^{-1}may be regarded as two vibrations in which the atoms move along the bond axis. In other words, these two frequencies are due to stretching mode of vibrations. Symmetric vibrations give rise to polarised Raman lines and asymmetric vibrations to depolarised Raman lines. Hence, the frequency 1285 cm^{-1} is due to symmetric stretching, while that at 2224 cm^{-1} is due to asymmetric stretching. The frequency 589 cm^{-1} shows a PQR branch and so it must be perpendicular mode of vibration.