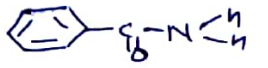
IR Spectra of Amides

(PRIMARY and N-SUBSTITUTED)

Amongst primary aliphatic amides only $HCONH_2$ is the liquid at room temperature, all the others are solids. Amides have the maximum extent of H-bonding amongst organic functional groups (i.e they have four degrees of H-bonding) N-N-Disubstituted amides are also solids except $HCONMe_2$, $HCONEt_2$.) 

The Infrared spectrum of Benzamide shows the very characteristic pair of bands for N—H str. near 3200 and 3400 cm^{-1}, the separation between these bands in the solid-state spectra (120-180 cm^{-1}) is usually sufficient to identify primary amides.

The primary amides in very dilute solution give N—H str near 3400 and 3500 cm^{-1}. secondary near 3450 cm^{-1}. and tertiary gives no such band as it does not possess any N—H bond. N-H str frequencies shift with concentrations

C=O str and N—H def, being coupled vibrations gives rise to bands that are named as amide I and amide II bands: respectively near 1650 cm^{-1}! This double band is also highly characteristic of amide. The higher frequency band is predominantly C=O str, and the lower is predominantly N—H def. Other amide bands of mixed assignment are named III, IV, V and VI. like C—N str.

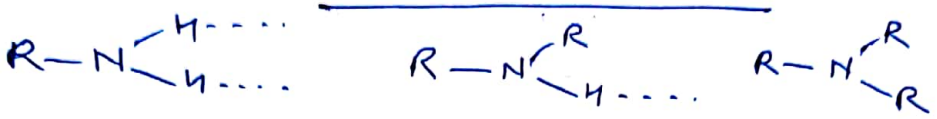
The amides have C—N bond with

(a) double bond character due to the mesomeric effect  . This may lead to geometrical Isomerism and cis and trans forms,

(b) the degree of vibrational coupling that takes place (N—H str may couple both N-H str & N-def) NH def couples strongly with C=O and C—N str.

These factors H-bonding due to association, cis trans isomerism and vibrational coupling lead to many absorptions and donot simply it.

IR SPECTRA of AMINES



Hydrogen bonding in amines lead to modification of both the symmetric and antisymmetric N–H str bands but shifts on dilution are less than for O–H str in alcohols and phenols. In dilute solution free N–H str can be observed at 3500 cm^{-1}.

The IR spectra of o-toluidine shows N–H str (two bands 3440 cm^{-1}) N–H def. at 1620 cm^{-1} and CN-str. at 1280 cm^{-1}.

IR SPECTRA for –C≡N.

The easiest to be detected by a strong band at 2250 cm^{-1} for C≡N str.

Reference Books

1. organic spectroscopy by William Kemp.