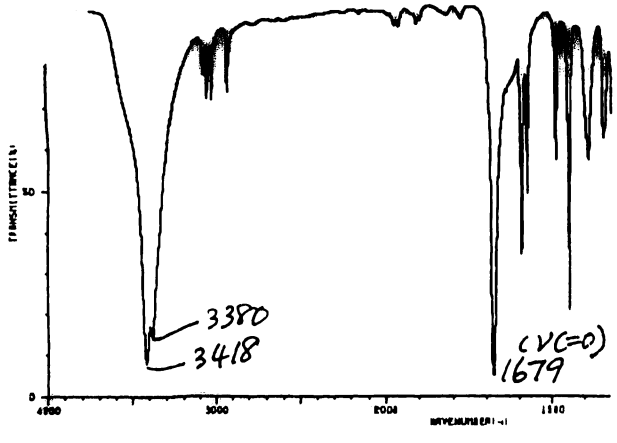
Website for spectroscopic data:
SDBS (Spectral Database for Organic Compounds) site:
http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng

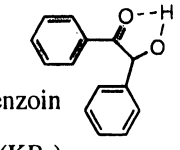
Important IR Peaks

• "***Use only the 4000 – 1430 cm^{-1} region.***" This is where most of the characteristic stretching vibration absorptions appear.

I. 4000 – 3100 cm^{-1}

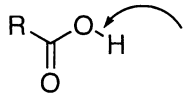
(1) νO-H: 3600 ~ 3200 cm^{-1} – *broad and very strong*
• Intermolecular H-bonding → lower cm^{-1}
3600 ~ 3500 cm^{-1}: dimeric; 3400 ~ 3200 cm^{-1}: polymeric
• Intramolecular H-bonding → lower cm^{-1} & sharper OH band





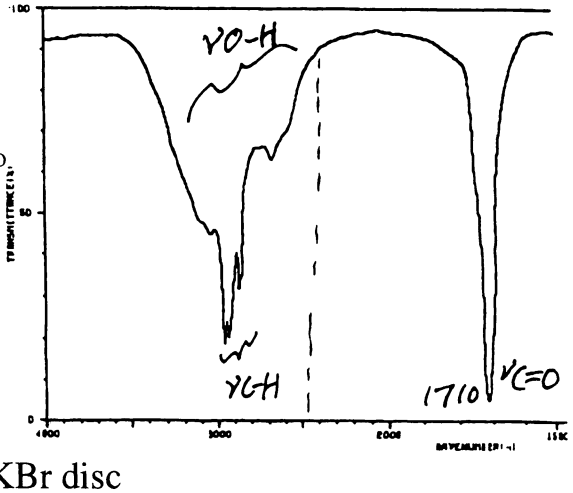
benzoin
(KBr)

Note:

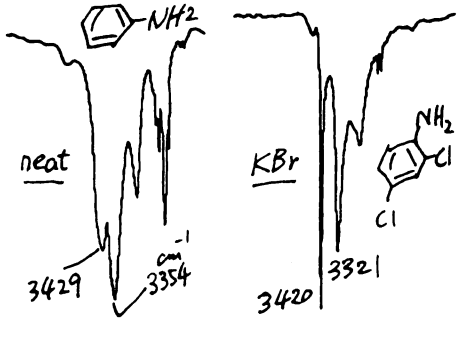


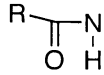
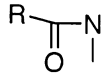
3400 ~2500 cm^{-1} (extremely broad νOH) due to extensive intermol. H-bonding (polymeric)

$CH_3(CH_2)_4COOH$ (neat)



(2) νN-H: 3500 ~ 3300 cm^{-1} – less broad than νOH; medium to strong intensity;
R-NH_2 shows two peaks due to the coupling of the two N-H dipoles - broad when run neat; sharper when run as a KBr disc



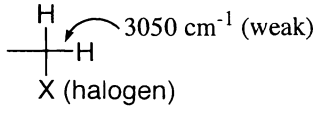
-  2°-amine; νNH weaker
-  1°-amide; ~3500 & ~3400 cm^{-1} often several bands in 3200~3050 cm^{-1}
-  2°-amide; 3460 ~3400 cm^{-1}; two bands; only one band with lactams

(3) ν ≡C-H: 3310~3200 cm^{-1} – strong; should also see ν C≡C (2140~2100 cm^{-1})

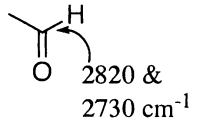
II. 3100 ~ 2700 cm^{-1}: νC-H (medium to weak intensity)

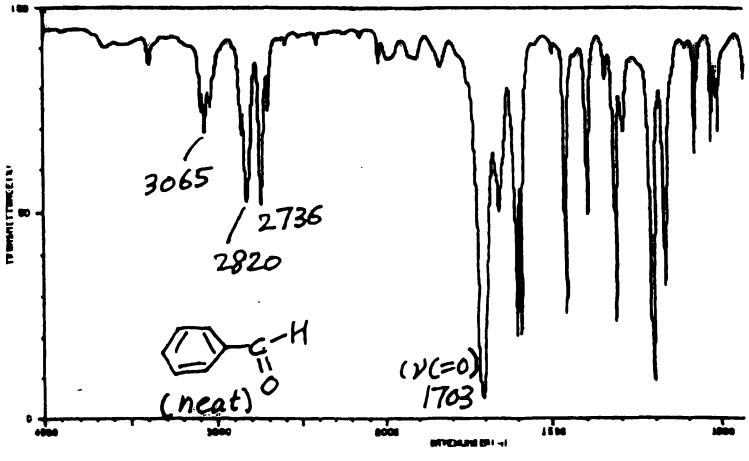
- aromatic and alkenic νC-H: 3100~3010 cm^{-1}
- alkanic (sp^3) νC-H: 2960~2850 cm^{-1}

Note:



Aldehydes:





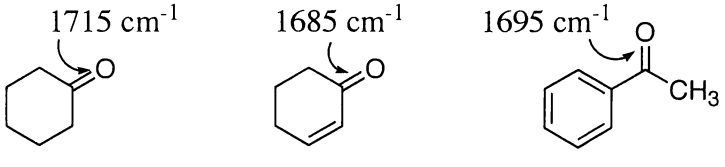
III. 2260 ~ 2100 cm^{-1}:
νC≡C, νC≡N, νC=C=C
sharp but weak

note: The two peaks you get in your IR spectra at ~2350 are due to νO=C=O of CO_2 present in the air.

IV. 1850 ~ 1620 cm^{-1}: various νC=O; ***very strong***

- acid anhydrides: 1850~1800 **and** 1790~1740 cm^{-1} (two peaks)
- acid halides: 1830~1780 cm^{-1}
- esters and six-membered lactones: 1750~1735 cm^{-1}
- aldehydes: 1730~1720 cm^{-1} (slightly higher cm^{-1} than corresponding ketone νC=O
- ketones: 1715 cm^{-1} (1720~1705 cm^{-1})
- carboxylic acid: 1720~1700 cm^{-1}
- amides: 1680~1640 cm^{-1}

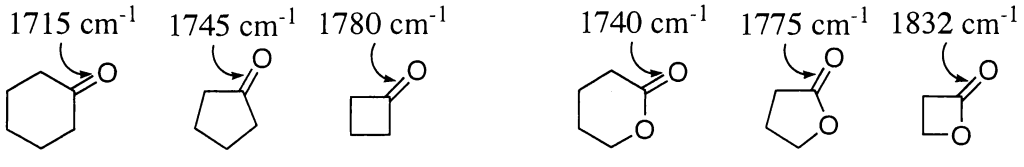
Notes:
(1) Conjugation lowers νC=O by 30~20 cm^{-1}



α,β-unsaturated ketone

aryl ketone

(2) Ring strain raises νC=O



V. 1680 ~ 1500 cm^{-1}: various νC=C (intensity variable) & νC=N (***strong***)

Arom νC=C: often 2~3 or more bands at ~1600, 1500, 1400 cm^{-1}; can be very strong