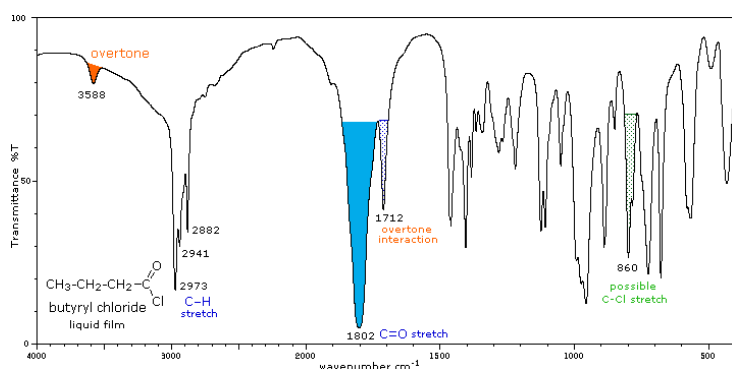


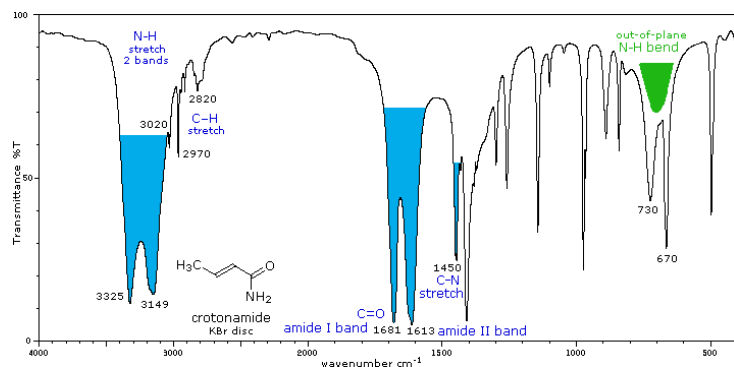
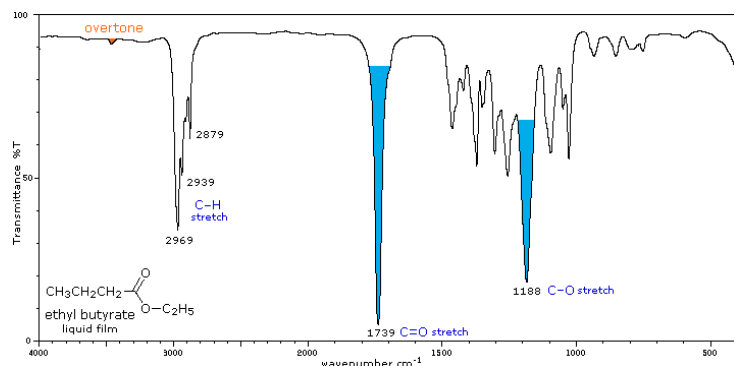
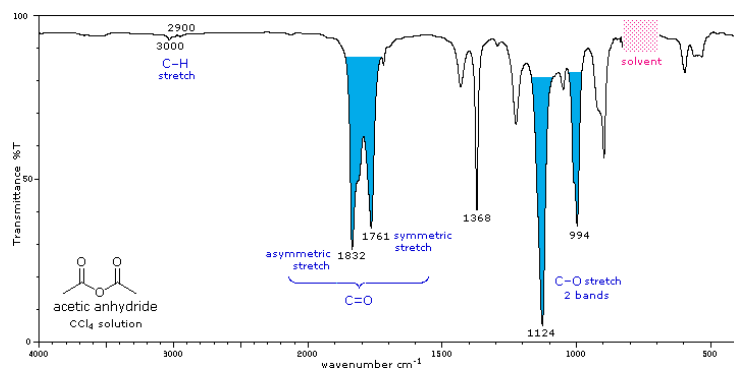
## 20.14: Spectroscopic Properties

The influence of heteroatom substituents on the reactivity of carbonyl functions toward nucleophiles was discussed earlier with respect to [carboxylic acid derivatives](#). A useful relationship exists between the reactivity of these derivatives and their carbonyl stretching frequencies. Thus, the very reactive acyl halides and anhydrides absorb at frequencies significantly higher than ketones, whereas the relatively unreactive amides absorb at lower frequencies. These characteristics are listed below.

Infrared spectra of many carboxylic acid derivatives will be displayed in the figure below the table by clicking the appropriate buttons presented there.

Carbonyl Derivative	Carbonyl Absorption	Comments
<b>Acyl Halides (RCOX)</b> X = F X = Cl X = Br	<b>C=O stretch</b> $1860 \pm 20 \text{ cm}^{-1}$ $1800 \pm 15$ $1800 \pm 15$	<a href="#">Conjugation lowers the C=O frequencies reported here, as with aldehydes &amp; ketones.</a> In acyl chlorides a lower intensity shoulder or peak near $1740 \text{ cm}^{-1}$ is due to an overtone interaction.
<b>Acid Anhydride, (RCO)<sub>2</sub>O</b> acyclic 6-membered ring 5-membered ring	<b>C=O stretch (2 bands)</b> $1750 \text{ & } 1820 \text{ cm}^{-1}$ $1750 \text{ & } 1820$ $1785 \text{ & } 1865$	<a href="#">Conjugation lowers the C=O frequencies reported here, as with aldehydes &amp; ketones.</a> The two stretching bands are separated by $60 \pm 30 \text{ cm}^{-1}$ , and for acyclic anhydrides the higher frequency (asymmetric stretching) band is stronger than the lower frequency (symmetric) absorption. Cyclic anhydrides also display two carbonyl stretching absorptions, but the lower frequency band is the strongest. One or two -CO-O-CO- stretching bands are observed in the $1000 \text{ to } 1300 \text{ cm}^{-1}$ region.
<b>Esters &amp; Lactones (RCOOR')</b> esters 6-membered lactone 5-membered lactone 4-membered lactone	<b>C=O stretch</b> $1740 \text{ cm} \pm 10 \text{ cm}^{-1}$ $1740 \text{ cm} \pm 10$ $1765 \text{ cm} \pm 5$ $1840 \text{ cm} \pm 5$	<a href="#">Conjugation lowers the C=O frequencies reported here, as with aldehydes &amp; ketones</a> Strong CO-O stretching absorptions (one or two) are found from $1150 \text{ to } 1250 \text{ cm}^{-1}$
<b>Amides &amp; Lactams (RCONR<sub>2</sub>)</b> 1° & 2°-amides 3°-amides 6-membered lactams 5-membered lactams 4-membered lactams	<b>C=O bands</b> $1510 \text{ to } 1700 \text{ cm}^{-1}$ (2 bands) $1650 \pm 15$ (one band) $1670 \pm 10$ (one band) $1700 \pm 15$ $1745 \pm 15$	<a href="#">The effect of conjugation is much less than for aldehydes &amp; ketones.</a> The higher frequency absorption ( $1665 \pm 30$ ) is called the <b>Amide I band</b> . The lower frequency <b>Amide II band</b> ( $1620 \pm 30$ in 1° amides & $1530 \pm 30$ in 2° amides) is largely due to N-H bending trans to the carbonyl oxygen. In concentrated samples this absorption is often obscured by the stronger amide I absorption. Hydrogen bonded association shifts some of these absorptions, as well as the prominent N-H stretching absorptions. <b>N-H stretch:</b> $3170 \text{ to } 3500 \text{ cm}^{-1}$ . Two bands for 1°-amides, one for 2°-amides.





## NMR Spectra

Protons on carbons adjacent to carbonyls absorb at ~2.0-2.5 ppm.

The N-H protons attached to primary and secondary amines absorb at ~7.5-8.5.

The carbonyl carbon in carboxylic acid derivatives show up at ~ 160-180 ppm.

The carbon in a nitrile appear ~ 115-120 ppm in their <sup>13</sup>C NMR spectrum. This is because of their *sp* hybridization.

## Contributors

- William Reusch, Professor Emeritus ([Michigan State U.](#)), [Virtual Textbook of Organic Chemistry](#)

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