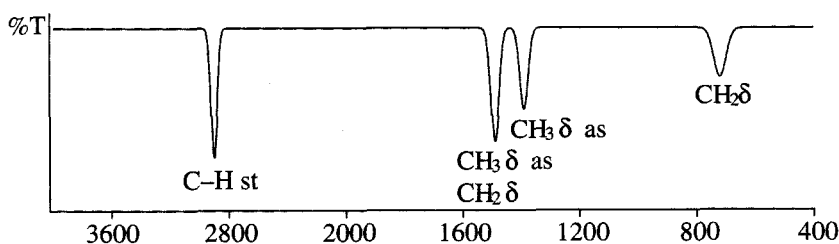






## 6 IR Spectroscopy



### 6.1 Alkanes



#### *Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )*

Assignment	Range	Comments
<b>C-H st</b>	3000–2840	Intensity variable, often multiplet
	<i>Beyond normal range:</i>	
	2850–2815	CH <sub>3</sub> –O, methyl ethers
	2880–2830	CH <sub>2</sub> –O, ethers
	2880–2835, 2780–2750	O–CH <sub>2</sub> –O, methylenedioxy
	≈2820	O–CH–O, acetals: weak
	3050–3000	 O,  N
	2900–2800, 2780–2750	CH=O, aldehydes: Fermi resonance
	2820–2780	CH <sub>3</sub> –N, CH <sub>2</sub> –N; amines
	3100–3050, 3035–2995	
	≈2700	 comb for cyclohexanes (CH <sub>2</sub> as st ≈2930)
	3080–2900	CH–hal



Assignment	Range	Comments
<b>CH<sub>3</sub> δ as</b>	1470–1430	Medium, coincides with CH <sub>2</sub> δ
	<i>Beyond normal range:</i>	
	1440–1400	CH <sub>3</sub> –C=O, methyl ketones, acetals CH <sub>3</sub> –C=C
<b>CH<sub>2</sub> δ</b>	1475–1450	Medium, coincides with CH <sub>3</sub> δ as
	<i>Beyond normal range:</i>	
	≈1440	CH <sub>2</sub> –C=C CH <sub>2</sub> –C≡C
	≈1425	CH <sub>2</sub> –C=O, CH <sub>2</sub> –C≡N, CH <sub>2</sub> –X (X: hal, NO <sub>2</sub> , S, P)
<b>CH<sub>3</sub> δ sy</b>	1395–1365	Medium. Doublet in compounds with geminal methyl groups:
	≈1385, ≈1370	CH(CH <sub>3</sub> ) <sub>2</sub> , equal intensity (γ: 1175–1140, d)
	≈1385,	C(CH <sub>3</sub> ) <sub>2</sub> , 1385 weaker than 1365
	≈1365	(γ: 1220–1190, often d)
	≈1390,	C(CH <sub>3</sub> ) <sub>3</sub> , of equal intensity, sometimes triplet
	≈1365	(γ: 1250–1200, d) N(CH <sub>3</sub> ) <sub>2</sub> , no doublet
		Solid-state spectra: sometimes doublet also in the absence of geminal methyl groups
	<i>Beyond normal range:</i>	
	1325–1310	SO <sub>2</sub> –CH <sub>3</sub>
	1330–1290	S–CH <sub>3</sub> , sulfides
	1310–1280	P–CH <sub>3</sub>
	1275–1260	Si–CH <sub>3</sub> , strong, sharp
<b>CH<sub>3</sub> γ</b>	1250–800	Intensity variable, of no practical significance Strong band in compounds with geminal methyl groups:
	1175–1140	CH(CH <sub>3</sub> ) <sub>2</sub> , doublet
	1220–1190	C(CH <sub>3</sub> ) <sub>2</sub> , generally doublet
	1250–1200	C(CH <sub>3</sub> ) <sub>3</sub> , doublet, often not resolved
	<i>Beyond normal range:</i>	
	≈765	SiCH <sub>3</sub>
	≈855, ≈800	Si(CH <sub>3</sub> ) <sub>2</sub>
	≈840, ≈765	Si(CH <sub>3</sub> ) <sub>3</sub>

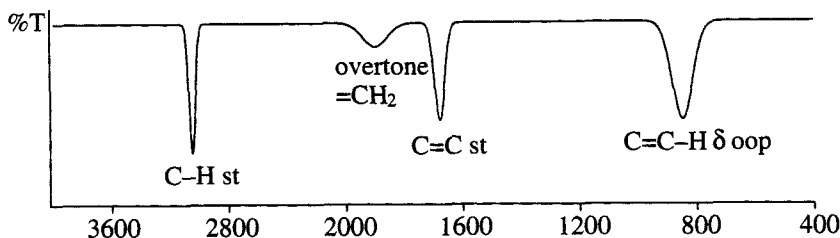
Assignment	Range	Comments
<b>CH<sub>2</sub></b> $\gamma$	770–720	Medium, sometimes doublet C–(CH <sub>2</sub> ) <sub>n</sub> –C for n > 4 at $\approx$ 720; for n < 4 at higher wavenumbers; in cyclohexanes at $\approx$ 890, weaker
	<i>Beyond normal range:</i> 1060–800	Cycloalkanes, numerous bands, unreliable
<b>C–D</b> $\sigma$	2200–2080	In general, substitution of L by isotope L': $\nu_{X-L'} = \nu_{X-L} \sqrt{\frac{1/m_X + 1/m_{L'}}{1/m_X + 1/m_L}}$



## 6.2 Alkenes










### 6.2.1 Monoenes






#### *Typical Ranges* ( $\nu$ in $\text{cm}^{-1}$ )




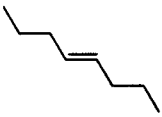
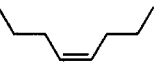

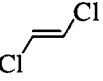

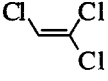

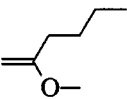
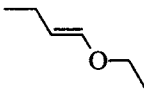
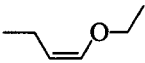
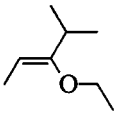
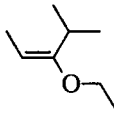
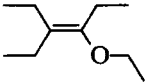
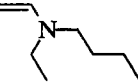
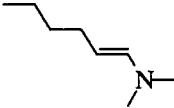
Assignment	Range	Comments
$=\text{CH}_2$ st	3095–3075	Medium, often multiple bands
$=\text{CH}$ st	3040–3010	Medium, often multiple bands CH st in aromatics and three-membered rings fall in the same range
<i>In cyclic compounds:</i>		
$\approx 3075$		
$\approx 3060$		
$\approx 3045$		
$\approx 3020$		
$=\text{CH}$ $\delta$ ip	1420–1290	Of no practical significance
$=\text{CH}$ $\delta$ oop	1005–675	A number of bands <i>In the same range also:</i> ar CH $\delta$ oop, C–O–C $\gamma$ , and C–N–C $\gamma$ in saturated heterocyclics, OH $\delta$ oop in carboxylic acids, NH $\gamma$ , NO st, SO st, CH <sub>2</sub> $\gamma$ , CF st, CCl st


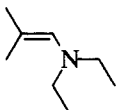


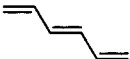

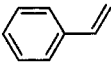

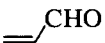



Assignment	Range	Comments			
<i>Subranges:</i>					
	C=C	C=C-C=O	C=C-OR	C=C-O-C=O	
CH=CH <sub>2</sub>	1005-985 920-900 (with overtone ≈810 at 1850-1800)	≈980 ≈960	≈960 ≈815	≈950 ≈870	C = C
C=CH <sub>2</sub>	900-880 (with overtone ≈810 at 1850-1780)	≈940	≈795		
	990-960	≈975	≈960	≈950	
	725-675	≈820			
	840-800	≈820			
C=C st	1690-1635	Of variable intensity, weak for highly symmetric compounds, strong for N=C=C and O=C=C			
<i>Subranges:</i>					
	1650-1635	CH=CH <sub>2</sub>			
	1660-1640	C=CH <sub>2</sub>			
	1690-1665		Weak		
	1665-1635				
	1690-1660		Weak, often absent		
	1690-1650		Weak, often absent		
<i>Beyond normal range:</i>					
	down to ≈1590	C=C-X with X: O, N, S; of higher intensity; in vinyl ethers often doublet due to rotational isomers			

At lower frequency if conjugated with:

C=C	C=C	≈1650		≈1630
		≈1600		
	C≡C	≈1600		≈1640
	C≡N	≈1620		≈1640
	C=O	≈1630		

**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )


	1645 994 912		1647 889 669		1682 972 963
	1670 968		1650 709		1667 825
	1575 826 761		1595 848 714		1587 929 835 780
	liquid: CCl <sub>4</sub> : 1610 1634 1608 987 964 810 943		1655 1592 958 793		1670 1652 937 925
	1663		1660		1673
	1663		1628		1650

	1640		1662		
	1652 1612		1830 1621 987 818		1800 1621 941 899
	1607 (2270)		1636		1645 1612
	1618 (1704)		1618 (1684)		1635 1615 (1730) (1706)
	1637 (1735)				

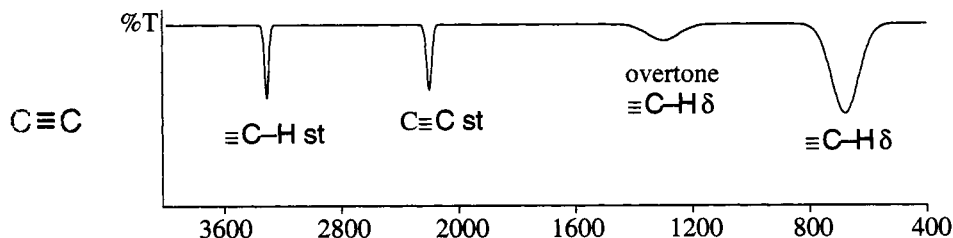
C=C

C=C

### 6.2.2 Allenenes

Assignment	Range	Comments
$(C=C)=C-H$ st	3050–2950	
$C=C=C$ st as	1950–1930	Strong, doublet in $X-C=C=CH_2$ if X other than alkyl Ring strain increases frequency:  $\approx 2020$
$C=C=C$ st sy	1075–1060	Weak, absent with highly symmetric substitution
$(C=C)=CH_2$ $\delta$ oop	$\approx 850$	Strong, overtone at $\approx 1700$ , weak

### 6.3 Alkynes



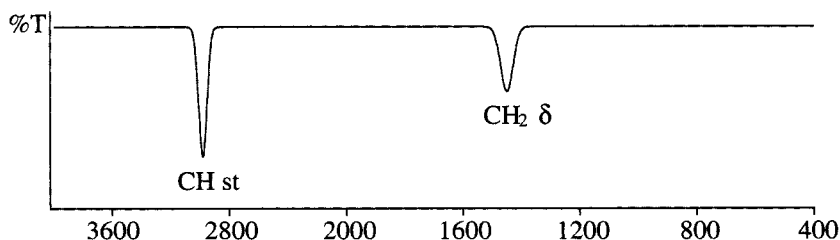
#### *Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )*

Assignment	Range	Comments
$\equiv\text{C-H}$ st	3340–3250	Strong, sharp; in the same region also OH st, NH st
$\text{C}\equiv\text{C}$ st	2260–2100	Weak, sharp
<i>Beyond normal range:</i>		
		$\text{R-C}\equiv\text{C-H}$ ; at the lower end of the cited range
		$\text{R-C}\equiv\text{C-R}$ ; usually 2 bands (Fermi resonance), often missing if symmetrical
<i>Subranges:</i>		
	$\approx 2120$	$\text{C-C}\equiv\text{C-H}$
	$\approx 2220$	$\text{C-C}\equiv\text{C-C}$
	$\approx 2240$	$\text{C-C}\equiv\text{C-CN}$
	$\approx 2240$	$\text{C-C}\equiv\text{C-COOH}$
	$\approx 2240, \approx 2140$	$\text{C-C}\equiv\text{C-COOCH}_3$
<i>In the same range: <math>\text{C}\equiv\text{Z}</math> st, <math>\text{X=Y=Z}</math> st, <math>\text{Si-H}</math> st</i>		
$\equiv\text{C-H}$ $\delta$	700–600	Strong, broad; overtone at 1370–1220 (broad, weak)

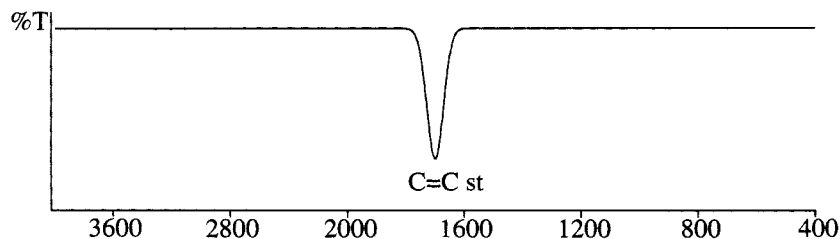


## 6.4 Alicyclics

### *Cyclic Alkanes*



### *Cyclic Alkenes*

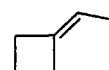
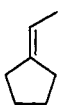
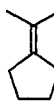
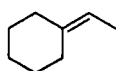
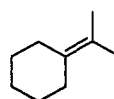


The other vibrations are similar to those in noncyclic alkenes and cyclic alkanes.

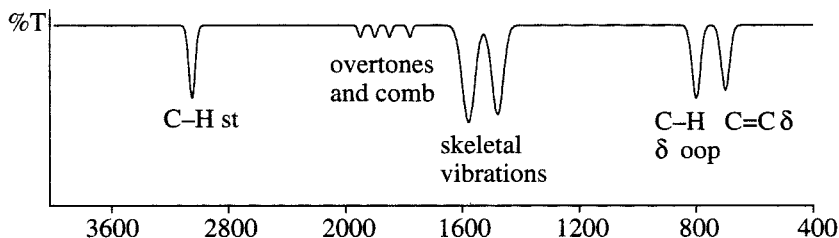
### *Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )*

Assignment	Range	Comments
<b>C-H st</b>	3090–2860	Strong
<b>H-C-H <math>\delta</math></b>	1470–1430	Weak
<b>C=C st</b>	1780–1610	Varies with ring size and substitution


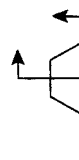
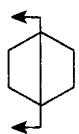

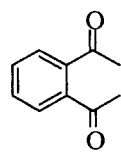
Twisting and wagging CH<sub>2</sub> as well as C-C st do not significantly differ from the corresponding vibrations in noncyclic compounds and are of limited diagnostic value.

**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )3090  
3019  
2933  
14342974  
2896  
14502951  
2871  
14552920  
2860  
14472933  
2865  
14622941  
1471  
1451 $\approx 1640$  $\approx 1780$  $\approx 1650$  $\approx 1570$  $\approx 1640$  $\approx 1680$  $\approx 1690$  $\approx 1610$  $\approx 1660$  $\approx 1660$  $\approx 1670$  $\approx 1690$  $\approx 1570$  $\approx 1650$  $\approx 1675$  $\approx 1650$  $\approx 1665$  $\approx 1670$  $\approx 1615$

## 6.5 Aromatic Hydrocarbons



### Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )

Assignment	Range	Comments
<b>arC-H st</b>	3080–3030	Often numerous bands; in the same range also CH st of alkenes and small rings
<b>arC-C</b>	1625–1575	  <p>Medium, often doublet; generally weak in benzene derivatives having a center of symmetry in the ring</p> <p><i>In the same range also:</i> C=C st, C=N st, C=O st, N=O st, C-C in heterocyclics, NH <math>\delta</math></p>
	1525–1475	<p>Medium, often doublet:</p>   <p>Weak in:</p>  <p><i>In the same range:</i> C=O st, N=O st, C-C in heterocyclics, B-N st, CH<sub>3</sub> <math>\delta</math>, CH<sub>2</sub> <math>\delta</math>, NH <math>\delta</math></p>
<b>comb</b>	2000–1650	<p>Very weak; useful for determining substitution patterns in 6-membered aromatic rings</p> <p><i>In the same range also:</i> C=O st, B-H<math>\cdots</math>B st, N<sup>+</sup>-H st, H<sub>2</sub>O <math>\delta</math></p>



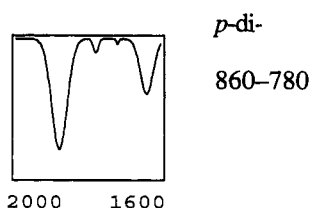
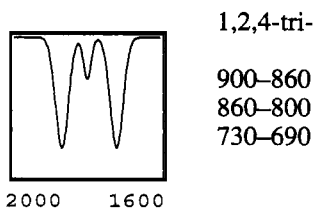
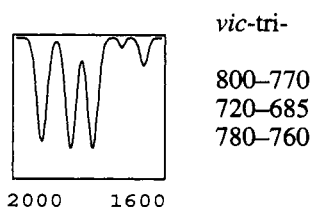
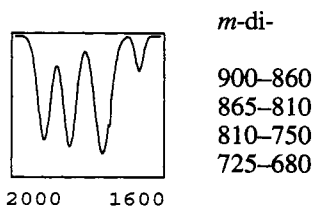
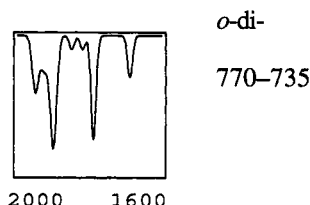
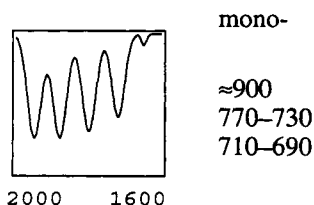
Assignment	Range	Comments
<b>arC-H <math>\delta</math> ip</b>	1250-950	Numerous bands of variable intensity; of no practical significance
<b>arC-H <math>\delta</math> oop</b>	900-650	One or more strong bands; useful for determining substitution patterns in 6-membered aromatic rings
<i>In the same range also: =C-H <math>\delta</math> oop, C-O-C <math>\gamma</math> and C-N-C <math>\gamma</math> in saturated heterocyclics, OH <math>\delta</math> oop in carboxylic acids, NH <math>\delta</math>, N-O st, S-O st, CH<sub>2</sub> <math>\gamma</math>, C-F <math>\delta</math>, C-Cl st</i>		

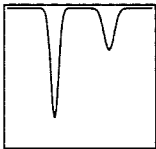
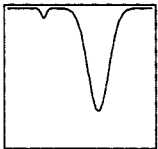
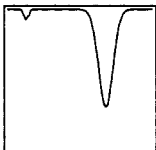
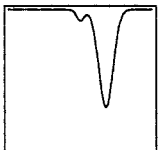
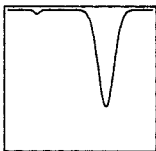
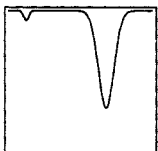


**Determination of Substitution Patterns in 6-Membered Aromatic Rings: Position and Shape of Bands Related to the Number of Adjacent H-Atoms ( $\nu$  in  $\text{cm}^{-1}$ )**

Not to be used for ring systems with strongly conjugated substituents such as C=O, NO<sub>2</sub>, C $\equiv$ N.

Comb, overtones	Substitution type; CH $\delta$ oop, ar C-C $\gamma$	Comb, overtones	Substitution type; CH $\delta$ oop, ar C-C $\gamma$
-----------------	--	-----------------	--



Comb, overtones	Substitution type; CH $\delta$ oop, ar C-C $\gamma$	Comb, overtones	Substitution type; CH $\delta$ oop, ar C-C $\gamma$
	1,2,3,4-tetra- 860–780		1,3,5-tri- 900–840 850–800 730–675
	1,2,3,5-tetra- 900–840		1,2,4,5-tetra- 900–840
	penta- 900–840		hexa- —



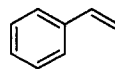
**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )



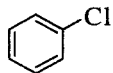
3080  
3040  
1968  
1818



3021  
1945  
1862  
1808  
1739



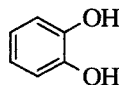
3086



3080



3040  
1915  
1845  
1775

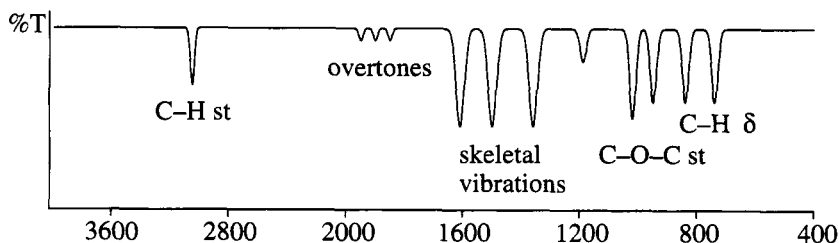


1927  
1887  
1764

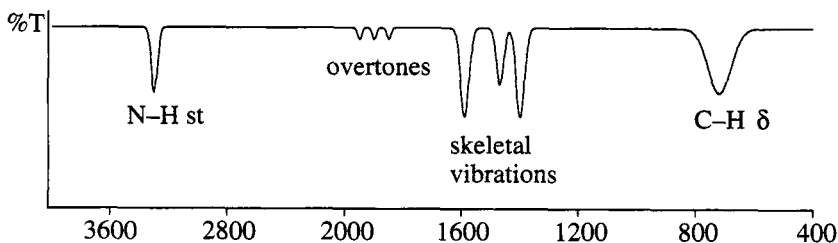
## 6.6 Heteroaromatic Compounds

*Characteristic Absorption Bands ( $\nu$  in  $\text{cm}^{-1}$ )*

### *Furans*






### *Pyrroles*



*Typical Ranges ( $\nu$  in  $\text{cm}^{-1}$ )*

Assignment	Range	Comments
<b>N-H st</b>	3450–3200	Medium, narrow; shifted by formation of hydrogen bonds
<b>Overtones</b>	2100–1800	Weak, characteristic
<b>Ring skeleton</b>	1610–1360	Strong, sharp bands
<b>C-H <math>\delta</math></b>	1000–700	Strong, broad; difficult to identify
<b>C-H st</b>	3100–3000	Medium, sharp
<b>CO-C st</b>	1190–990	Medium or strong; of variable intensity

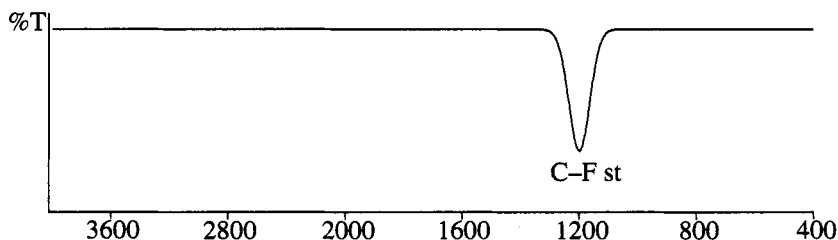
**5-Ring-Heteroaromatics:**

			
NH st free		3500–3400	
NH st H-bonded		3400–2800	
CH st	≈3100	≈3100	≈3100
Ring skeleton: intensity	1610–1560	1590–1560	1535–1515
variable, generally multiplets	1510–1475	1540–1500	1455–1410
CH $\delta$ oop: generally strong	990–725	770–710	935–700



## 6.7 Halogen Compounds

### 6.7.1 Fluoro Compounds

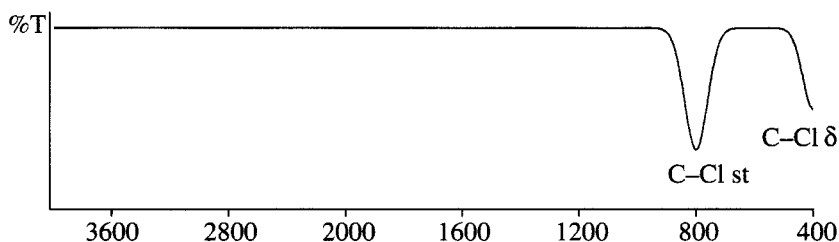


#### *Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )*

Assignment	Range	Comments
Hal C-F st	1400–1000	Strong, often more than one band (rotational isomers), often not resolved
	<i>Subranges:</i>	
	1100–1000	al $\text{CF}_2$ (FC-H st: 3080–2990)
	1150–1000	al $\text{CF}_2$
	1350–1100	al $\text{CF}_3$
	1350–1150	C=CF
	$\approx 1745$	C=CF <sub>2</sub> st
	1250–1100	ar CF
	<i>In the same range:</i> strong bands for C–O st, NO <sub>2</sub> st sym, C=S st, S=O st	
CF <sub>2</sub>	780–680	Medium or weak, assignment uncertain
CF <sub>3</sub>	780–680	(C–F $\delta$ ?)
S–F st	815–755	Strong
P–F st	1110–760	
Si–F st	980–820	
B–F st	1500–800	



### 6.7.2 Chloro Compounds

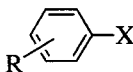


#### Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )

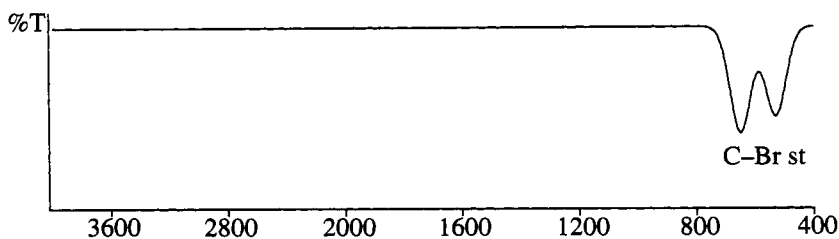
Assignment	Range	Comments
C-Cl st	1100–1020	Strong, narrow or of medium width; chloroaromatics
	830– <600	Strong, often broad (rotational isomers), absent in chloroaromatics
C-Cl $\delta$	400–280	Of medium strength and width
P-Cl st	<600	
Si-Cl st	<625	
B-Cl st	1100–650	

Hal

In disubstituted halobenzenes, characteristic skeletal vibrations:

	X	<i>ortho</i>	<i>meta</i>	<i>para</i>
	Cl	1055–1035	1080–1075	1095–1090
	Br	1045–1030	1075–1065	1075–1070
	I			1060–1055

### 6.7.3 Bromo Compounds

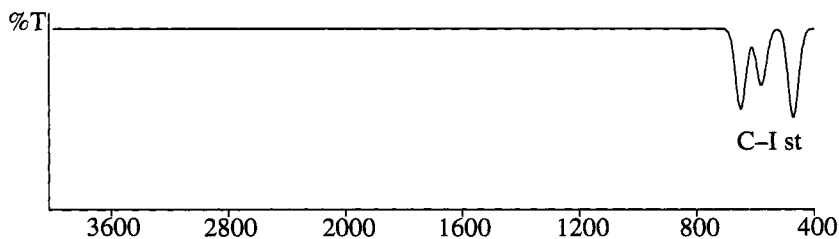


#### *Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )*

Assignment	Range	Comments
C-Br st	1080–1000	Strong, narrow or of medium width; bromoaromatics
	700–500	Strong, of medium width; absent in bromoaromatics
C-Br $\delta$	350–250	Of medium strength and width

Hal

### 6.7.4 Iodo Compounds



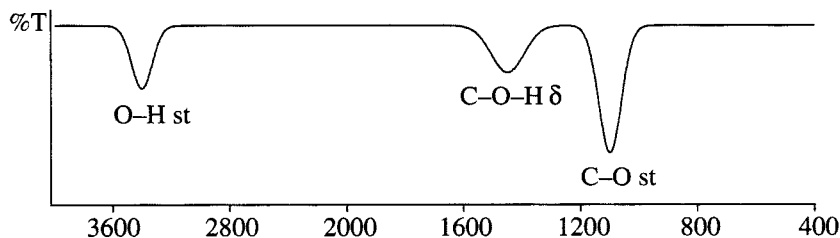
#### *Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )*

Assignment	Range	Comments
C-I st	650–450	Strong, two or more bands
C-I $\delta$	300–50	Of medium strength and width

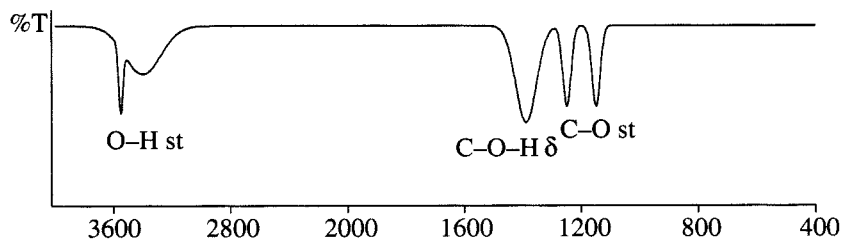
## 6.8 Alcohols, Ethers, and Related Compounds

### 6.8.1 Alcohols and Phenols

#### *Alcohols*



#### *Phenols*

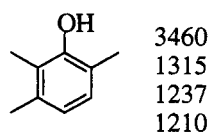
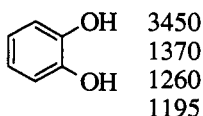
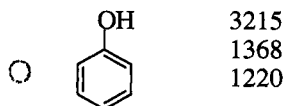
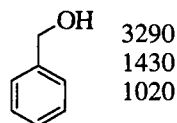
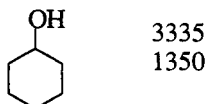
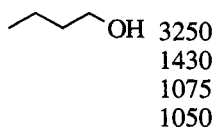


#### *Typical Ranges* ( $\nu$ in $\text{cm}^{-1}$ )

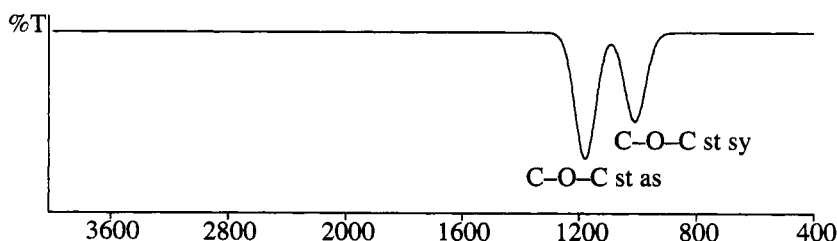
Assignment	Range	Comments
<b>O-H st</b>	3650–3200	Of variable intensity
	<i>Subranges:</i>	
	3650–3590	Free OH; sharp
	3550–3450	Hydrogen bonded OH; broad
	3500–3200	Polymer OH; broad, often numerous bands
	<i>Beyond normal range:</i>	
	3200–2500	Enols, chelates; often very broad
	<i>In the same range also:</i> NH st, $\equiv\text{CH}$ st ( $\approx 3300$ , sharp), $\text{H}_2\text{O}$	
<b>O-H δ ip</b>	1450–1200	Medium, of no practical significance

Assignment	Range	Comments
<b>C-O st</b>	1260–970	Strong, often doublet
	<i>Subranges:</i>	
	1075–1000	CH <sub>2</sub> -OH
	1125–1000	CH-OH
	1210–1100	C-OH
	1275–1150	ar C-OH
	<i>In the same range:</i> bands for C-F st, C-N st, N-O st, P-O st, C=S st, S=O st, P=O st, Si-O st, Si-H $\delta$	
<b>O-H <math>\delta</math> oop</b>	<700	Medium, of no practical significance

**Examples ( $\nu$  in  $\text{cm}^{-1}$ )**



### 6.8.2 Ethers, Acetals, Ketals






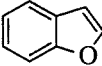


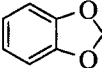


In acetals and ketals, the C–O stretching vibrations are split into 3, sometimes even 4 to 5 bands.

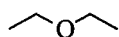
Acetals have an additional band due to a special C–H  $\delta$  vibration.

The C–H st vibration frequency is especially low: OCH<sub>3</sub> st, 2850–2815;

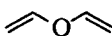
OCH<sub>2</sub> st, 2880–2835.

*Typical Ranges* ( $\nu$  in  $\text{cm}^{-1}$ )

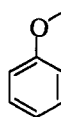
Assignment	Range	Comments
<b>C–O–C st as</b>	1310–1000	Strong, sometimes split
	<i>Subranges for non-cyclic ethers:</i>	
	1150–1085	$\text{CH}_2\text{--O--CH}_2$
	1170–1115	$\text{CH--O--CH}$ , often split
	1225–1180	$\text{C=C--O--alC}$
	1275–1200	$\text{arC--O--alC}$
	<i>Subranges for cyclic ethers:</i>	
	1280 sym	
	870 as	
	$\approx 1030$ sym	
	$\approx 980$ as	
	$\approx 1070$ sym	
	$\approx 915$ as	
	$\approx 1235$	
	$\approx 1100$ as	
	$\approx 815$ sym	
	$\approx 950$	 ketals, acetals: 4 to 5 bands
	$\approx 925$	
	1024, 1086 as $\approx 880$ sym	
	$\approx 800$	 in acetals: st CH, $\approx 2820$ , weak
<b>C–O–C st sym</b>	1055–870	Strong, sometimes multiple bands
	<i>Subranges for non-cyclic ethers:</i>	
	1125–1080	$\text{C=C--O--alC}$ , medium
	1075–1020	$\text{arC--O--alC}$ , medium
	<i>In the same range: strong bands for C–O st, C–F st, C–N st, N–O st, P–O st, C=S st, S=O st, P=O st, Si–O st, Si–H <math>\delta</math></i>	

**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )

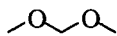
1136  
935  
917



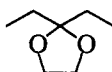
1225  
1218  
1211  
1003



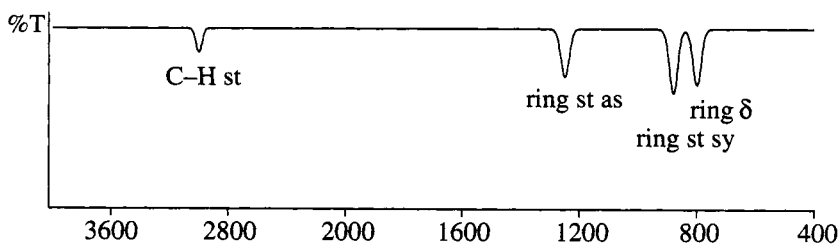
1250  
1040



1188  
1138  
1111  
1046



1172  
1132  
1077  
1057  
1038

**6.8.3  
Epoxides****Typical Ranges** ( $\nu$  in  $\text{cm}^{-1}$ )

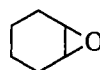
Assignment	Range	Comments
C-H st	3050–2990	Frequency higher than normally found in alkanes
ring st as	1280–1230	Variable intensity
ring st sy	950–815	Variable intensity
ring def	880–750	Variable intensity

**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )

1280  
870

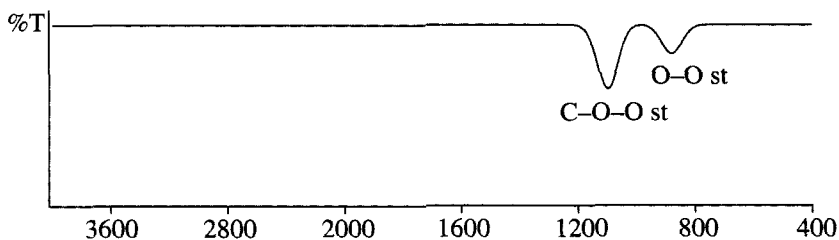


1230 sy  
885 as  
845  $\delta$



1260 sy  
890 as  
780  $\delta$

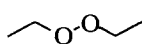
### 6.8.4 Peroxides and Hydroperoxides



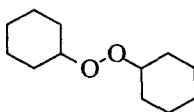
#### Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )

Assignment	Range	Comments
<b>O-O-H st</b>	3450–3200	Of variable intensity
	<i>Subranges:</i>	
	$\approx 3450$	Free OOH; H-bonded: $\approx 30 \text{ cm}^{-1}$ higher than in corresponding alcohols
		<i>In the same range:</i> OH st, NH st, $\equiv\text{CH}$ st, $\text{H}_2\text{O}$
<b>C-O-O st</b>	1200–1000	Strong, about $\approx 20 \text{ cm}^{-1}$ lower than in corresponding alcohols
		<i>In the same range:</i> strong bands for C-O st, C-F st, C-N st, N-O st, P-O st, C=S st, S=O st, P=O st, Si-O st, Si-H $\delta$
<b>O-O st</b>	1000–800	Medium or weak, often doublet, assignment uncertain
Also:	1760–1745	C=O st in peracids
	1820–1770	C=O st in diacylperoxides (two bands)

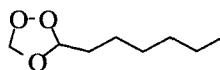
#### Examples ( $\nu$ in $\text{cm}^{-1}$ )



1017  
880



1070  
1060  
943

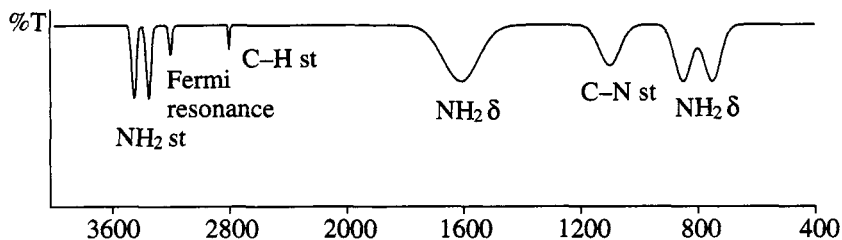


1100  
852

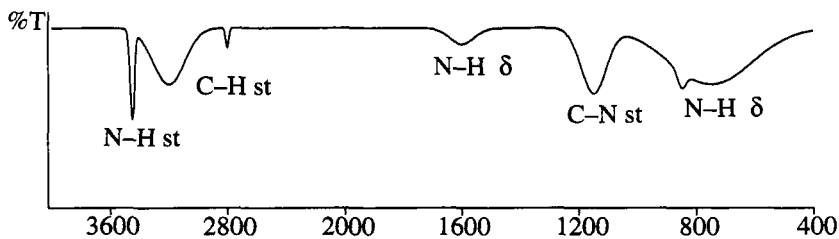
## 6.9 Nitrogen Compounds

### 6.9.1 Amines and Related Compounds

#### *Primary Amines*

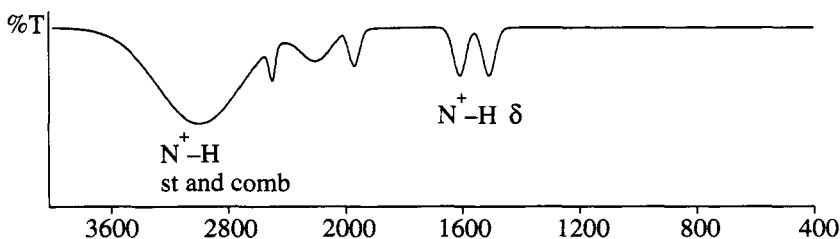


#### *Secondary Amines*



N

#### *Ammonium*





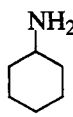
*Typical Ranges ( $\nu$  in  $\text{cm}^{-1}$ )*

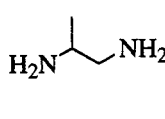
Assignment	Range	Comments
$\text{NH}_2$ st	3500–3300	Of variable intensity, generally 2 sharp bands, $\Delta\nu = 65\text{--}75$ At lower wavenumbers ( $<3200$ ) and broader if H-bonded. Free and H-bonded forms often simultaneously observed In primary aromatic amines additional combination band at $\approx 3200$ <i>In the same range:</i> OH st, $\equiv\text{CH}$ st
NH st	3450–3300	Of variable intensity, only one band At lower wavenumbers ( $<3200$ ) and broader if H-bonded. Free and H-bonded forms often simultaneously observed <i>In the same range:</i> OH st, $\equiv\text{CH}$ st, $\text{H}_2\text{O}$
$\text{NH}_3^+$ st	3000–2000 3000–2700	Medium, broad, highly structured Major maximum, comb: $\approx 2000$
$\text{NH}_2^+$ st	3000–2000 3000–2700	Medium, broad, highly structured Major maximum
$\text{NH}^+$ st	3000–2000 2700–2250	Medium, broad, highly structured Major maximum <i>In the same range:</i> OH st, NH st, CH st, SH st, PH st, SiH st, BH st, $\text{X}=\text{Y}=\text{Z}$ st, $\text{X}\equiv\text{Y}$ st
$\text{NH}_2$ $\delta$	1650–1590	Medium or weak
NH $\delta$	1650–1550	Weak
$\text{NH}_3^+$ $\delta$	1600–1460	Medium, often more than one band; weak in aliphatic amines
$\text{NH}_2^+$ $\delta$	1600–1460	Medium, often more than one band; weak in aliphatic amines
$\text{NH}^+$ $\delta$	1600–1460	Medium, often more than one band; weak in aliphatic amines
C–N st	1400–1000	Medium, of no practical significance
$\text{NH}_2$ $\delta$	850–700	Medium or weak; 2 bands in primary amines
NH $\delta$	850–700	Medium or weak
P–N–C st	1110–930, 770–680	

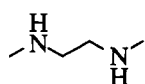
N

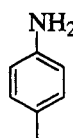
**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )

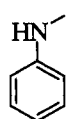
$\text{CH}_3\text{-NH}_2$     3470  
                   3360  
                   1622

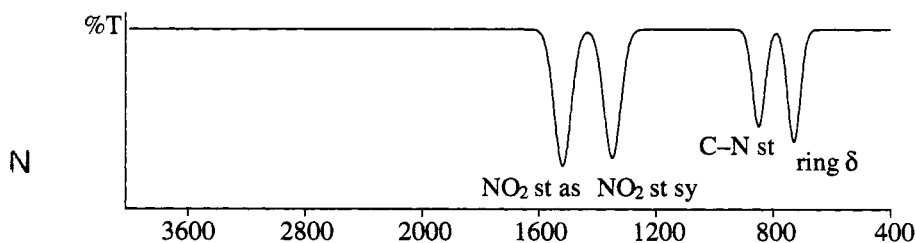
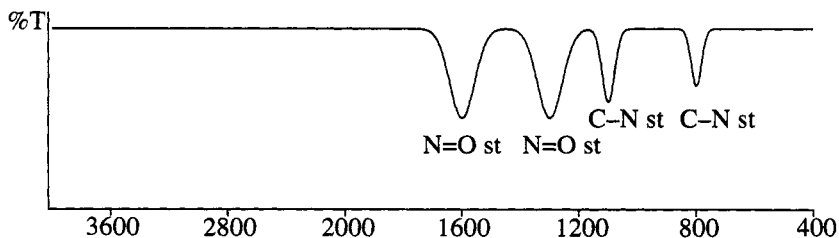
    3357  
                                  3278  
                                  3200 sh  
                                  1605

    3356  
                                  3274  
                                  3175  
                                  1650

    3279

    3487  
                                  3405

    3416  
                                  3386  
                                  1322  
                                  1266

**6.9.2****Nitro and Nitroso Compounds****Nitro Compounds****Nitroso Compounds**

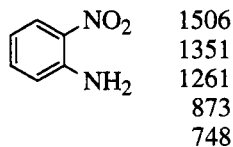
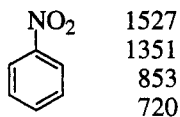
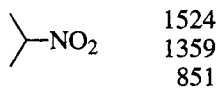
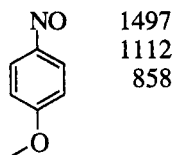
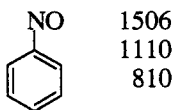
*Typical Ranges ( $\nu$  in  $\text{cm}^{-1}$ )*

Assignment	Range	Comments
<b>NO<sub>2</sub> st as</b>	1660–1490	Very strong, of medium width
	<i>Subranges:</i>	
	1660–1625	O–NO <sub>2</sub> , nitrates
	1570–1540	C–NO <sub>2</sub> , al nitro compounds
	1560–1490	C–NO <sub>2</sub> , ar nitro compounds
	1630–1530	N–NO <sub>2</sub> , nitramines
<b>NO<sub>2</sub> st sy</b>	1390–1260	Strong, of medium width
	<i>Subranges:</i>	
	1285–1270	O–NO <sub>2</sub> , nitrates
	1390–1340	C–NO <sub>2</sub> , al nitro compounds
	1360–1310	C–NO <sub>2</sub> , ar nitro compounds; often 2 bands
	1315–1260	N–NO <sub>2</sub> , nitramines
	<i>In nitrates also:</i>	
	≈870	N–O st, strong
	≈760	NO <sub>2</sub> $\gamma$
	≈700	NO <sub>2</sub> $\delta$
Ring $\delta$	760–705	Strong; modified deformation of aromatic ring
<b>N=O st</b>	1680–1450	Very strong, in monomers
	1420–1250	Very strong, in dimers
	<i>Subranges:</i>	
	1680–1650	O–NO (nitrites) <i>trans</i> ; 1625–1610: <i>cis</i>
	1585–1540	C–NO, al C-nitroso compounds
	1510–1490	C–NO, ar C-nitroso compounds
	≈1450	N–NO, <i>N</i> -nitroso compounds
	<i>In nitrites also:</i>	
	3300–3200, ≈2500, 2300–2250	comb
	≈800	N–O st <i>trans</i> ; <i>cis</i> : very weak
	≈600	O–NO $\delta$ <i>trans</i> ; <i>cis</i> : ≈650
<b>C–N st</b>	≈850	C–NO, al C-nitroso compounds; coupled with other vibrations
	≈1100	C–NO, ar C-nitroso compounds
<b>N–N st</b>	≈1040	<i>N</i> -Nitroso compounds

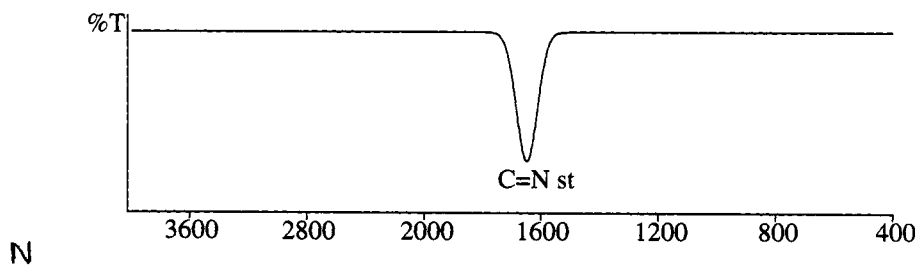
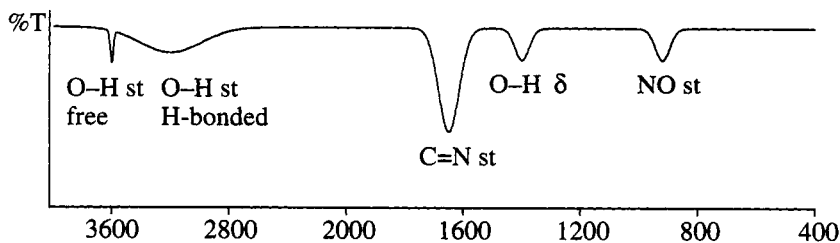
N

**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )

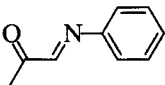
$\text{CH}_3\text{-NO}$       1564  
                    842



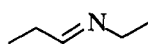
### 6.9.3 Imines and Oximes

**Imines****Oximes**

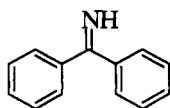
*Typical Ranges ( $\nu$  in  $\text{cm}^{-1}$ )*

Assignment	Range	Comments
<b>C=N st</b>	1690–1520	Generally strong
	<i>Subranges:</i>	
	$\approx 1670$	$\text{R}-\text{CH}=\text{N}-\text{R}'$ R, R': al
	$\approx 1645$	$\text{R}-\text{CH}=\text{N}-\text{R}'$ R or R': conjugated
	$\approx 1630$	$\text{R}-\text{CH}=\text{N}-\text{R}'$ R, R': conjugated
	$\approx 1655$	$\begin{array}{c} \text{R} \\ \diagdown \\ \text{C}=\text{N} \\ \diagup \\ \text{R}'' \end{array}$ R, R', R'': al
	$\approx 1645$	$\begin{array}{c} \text{R} \\ \diagdown \\ \text{C}=\text{N} \\ \diagup \\ \text{R}'' \end{array}$ R: conjugated
	$\approx 1635$	$\begin{array}{c} \text{R} \\ \diagdown \\ \text{C}=\text{N} \\ \diagup \\ \text{R}'' \end{array}$ R, R': conjugated
	$\approx 1555$	 additional band: $\approx 1655$ C=O
	$\approx 1645$	$\begin{array}{c} \text{R} \\ \diagdown \\ \text{C}=\text{NH} \\ \diagup \\ \text{R}' \end{array}$ R, R': al
	$\approx 1625$	$\begin{array}{c} \text{R} \\ \diagdown \\ \text{C}=\text{NH} \\ \diagup \\ \text{R}' \end{array}$ R, R': conjugated
	1685–1580	$\begin{array}{c} \text{R} \\ \diagdown \\ \text{C}=\text{N} \\ \diagup \\ \text{H}_2\text{N} \end{array}$ Additional band at 1540–1515 in: $\begin{array}{c} \text{R} \\ \diagdown \\ \text{C}=\text{N} \\ \diagup \\ \text{RHN} \end{array}$
	1670–1600	$\text{CH}=\text{N}-\text{N}=\text{CH}$
	1690–1645	$\begin{array}{c} \text{RO} \\ \diagdown \\ \text{C}=\text{NH} \\ \diagup \\ \text{RO} \end{array}$ Additional bands: NH st: $\approx 3300$ , C–O st: $\approx 1325$ , $\approx 1100$
	1680–1635	$\begin{array}{c} \text{RO} \\ \diagdown \\ \text{C}=\text{NH}_2^+ \\ \diagup \\ \text{RO} \end{array}$ Additional bands: $\text{NH}_2^+$ st: $\approx 3000$ , $\text{NH}_2^+$ $\delta$ : 1590–1540
	2050–2000	C=C=N; Ketimines, very strong, sometimes doublet
	1580–1520	Quinone oximes: C=O st 1680–1620
	1685–1650	Aliphatic oximes
	1645–1650	Aromatic oximes
	1690–1645	O–C=N
	1640–1605	S–C=N
	1640–1580	S–S–C=N
<b>OH st</b>	3600–2700	Strong
	<i>Subranges:</i>	
	$\approx 3600$	Free
	3300–3100	H-bonded, broad
	$\geq \approx 2700$	Quinone oximes, more than one band
<b>OH <math>\delta</math></b>	1475–1315	Of no practical significance
<b>N–O st</b>	1050–400	Of no practical significance

N

**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )

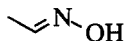
1667



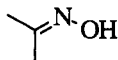
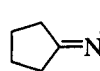
1603



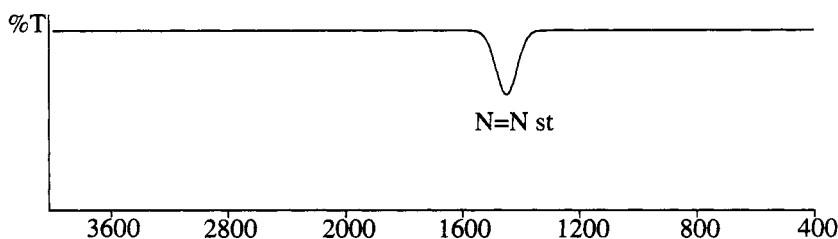
1637



1675

1672 (solid)  
1662 (gas)

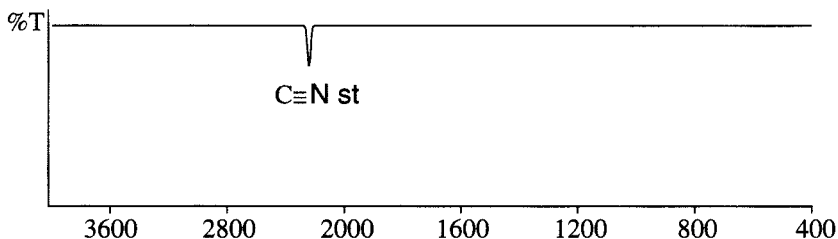
1684

**6.9.4**  
**Azo Compounds****Typical Ranges** ( $\nu$  in  $\text{cm}^{-1}$ )

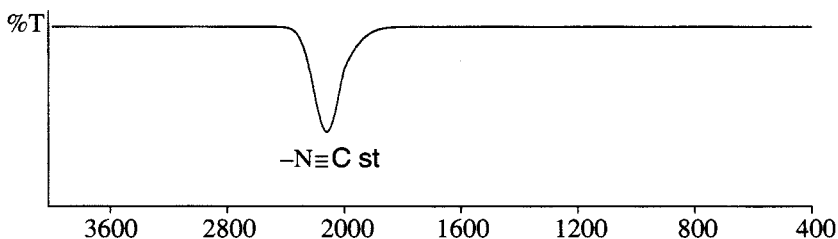
Assignment	Range	Comments
N	N=N st	1500–1400
		Very weak, missing in compounds of high symmetry
	1480–1450	 st as st sy
	1335–1315	
	≈1450	 
	≈1050	
	1410–1175	 Dimers of C-nitroso compounds
<i>Subranges:</i>		
	1290–1175	Aliphatic <i>trans</i>
	1425–1385, 1345–1320	Aliphatic <i>cis</i>
	1300–1250	Aromatic <i>trans</i>
	≈1410, ≈1395	Aromatic <i>cis</i>

### 6.9.5 Nitriles and Isonitriles

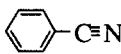
#### Nitriles



#### Isonitriles




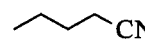
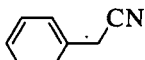
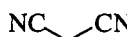
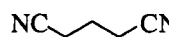
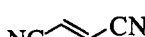
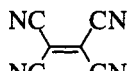
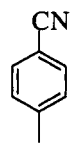
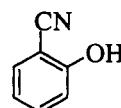
#### Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )

Assignment	Range	Comments
$\text{C}\equiv\text{N st}$	2260–2240	Medium to strong, sharp; for $\text{O}-\text{CH}_2-\text{C}\equiv\text{N}$ , $\text{N}-\text{CH}_2-\text{C}\equiv\text{N}$ : of low intensity or absent
	<i>Beyond normal range:</i>	
	2240–2215	$\text{C}=\text{C}-\text{C}\equiv\text{N}$
	2240–2215	
	2240–2230	$\text{XC}-\text{C}\equiv\text{N}$ X: Cl, Br, I
	$\approx 2275$	$-\text{CF}_2-\text{C}\equiv\text{N}$
	2225–2175	$\text{N}^+-\text{C}\equiv\text{N}^- \longleftrightarrow \text{N}^+=\text{C}=\text{N}^-$
	2210–2185	$>\text{N}-\text{C}=\text{C}-\text{C}\equiv\text{N}$
	2200–2070	$\text{C}\equiv\text{N}^-$
$-\text{N}^+\equiv\text{C}^-$	2150–2110	Strong

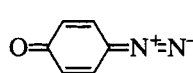
N

Assignment	Range	Comments
$\text{--N}^+\equiv\text{N}$	2310–2130	Medium, frequency depends on anion
<i>In the same range: C<math>\equiv</math>C st, X=Y=Z st as, NH<math>^+</math> st, PH st, POH st, SiH st, BH st</i>		

### Examples ( $\nu$ in $\text{cm}^{-1}$ )

	2222		2235		2252
	2273		2235		2252
	2257 2222		2245		2220
NaCN, KCN	2080–2070	AgCN	2178	NH $_2$ -CN	2268

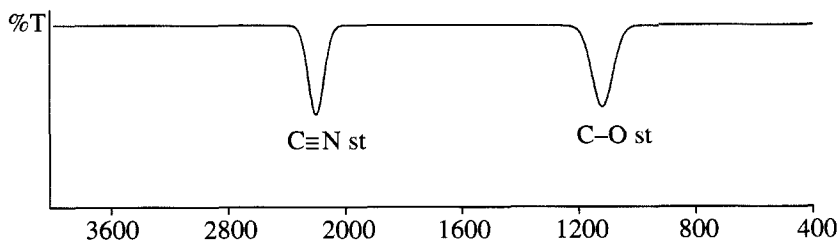
### 6.9.6 Diazo Compounds

Assignment	Range	Comments
$\text{N}^+\equiv\text{N}$ st	2310–2130	Medium, frequency depends on anion
$\text{C}=\text{N}^+=\text{N}^-$	2050–2010	Very strong
<i>Subranges:</i>		
	2050–2035	R-CH=N $^+$ =N $^-$ R: al or ar
	2035–2010	R $_2$ -C=N $^+$ =N $^-$ R: al or ar
<i>Beyond normal range:</i>		
	2100–2050	R-CO-C=N $^+$ =N $^-$ C=O st $\approx$ 1645 (R: al) C=O st $\approx$ 1615 (R: ar) C=N $^+$ =N $^-$ st sy: $\approx$ 1350, strong
	2180–2010	 C=O st 1655–1560

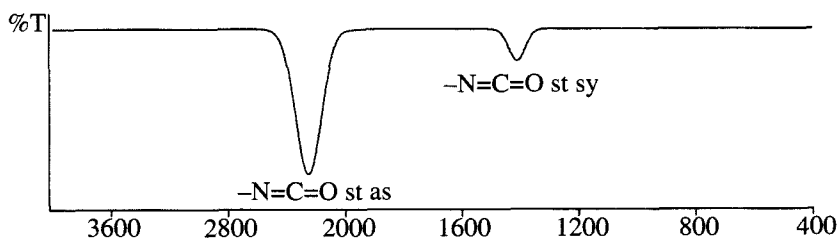


### 6.9.7 Cyanates and Isocyanates

#### Cyanates



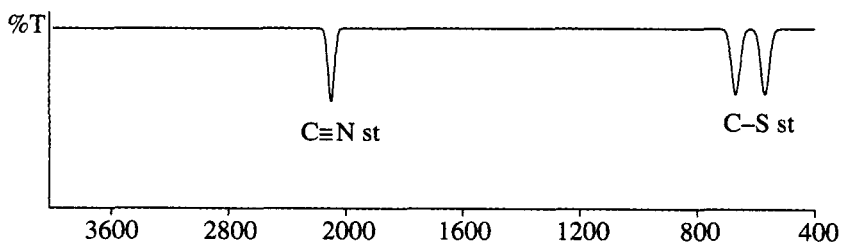
#### Isocyanates



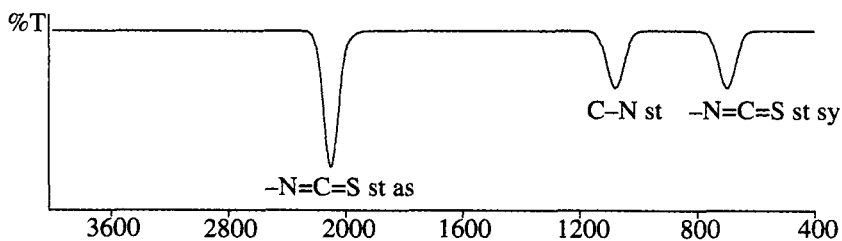
#### Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )

Assignment	Range	Comments
<b>OC≡N st</b>	2260–2130	Medium to strong
	2220–2130	(OC≡N) <sup>-</sup>
	1335–1290	(OC≡N) <sup>-</sup> st sy
<b>C–O st</b>	1200–1080	Strong
<b>N=C=O st as</b>	2280–2230	Strong, sharp
	≈2300	–CF <sub>2</sub> NCO
<b>N=C=O st sy</b>	1450–1380	Weak
	<i>Beyond normal range:</i>	
	2220–2130	(N=C=O) <sup>-</sup>

N

**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )CH3NCO 2265CCNCO 2280CC(C)NCO 2270C=CNCO 2256  
(1629 C=C)c1ccccc1NCO 2267CC(=O)NCO 2246**6.9.8****Thiocyanates and Isothiocyanates****Thiocyanates**

N

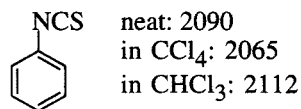
**Isothiocyanates**

**Typical Ranges** ( $\nu$  in  $\text{cm}^{-1}$ )

Assignment	Range	Comments
<b>SC<math>\equiv</math>N st</b>	2170–2130	Medium, sharp
	2090–2020	(SC $\equiv$ N) <sup>+</sup>
<b>C–S st</b>	750–550	Often doublet
<b>N=C=S st as</b>	2200–2050	Very strong, generally doublet, Fermi resonance
<b>N=C=S st sy</b>	950–650	
	$\approx$ 950	al –N=C=S
	700–650	ar –N=C=S
	<i>Beyond normal range:</i>	
	2090–2020	(N=C=S) <sup>+</sup>
<b>C–N st</b>	1090–1075	

**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )

CH <sub>3</sub> NCS	neat:	in CCl <sub>4</sub> :		NCS	2173
	2206				2097
	2114				2068
					2077



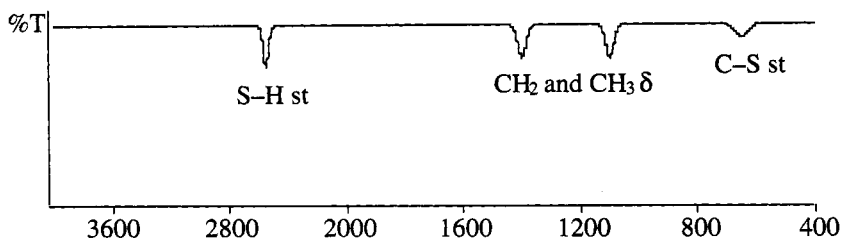
N

## 6.10

## Sulfur-Containing Functional Groups

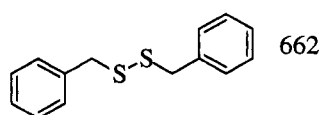
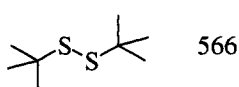
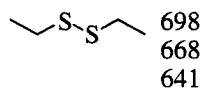
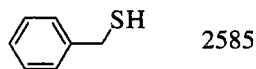
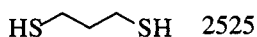
## 6.10.1

## Thiols and Sulfides

*Typical Ranges* ( $\nu$  in  $\text{cm}^{-1}$ )

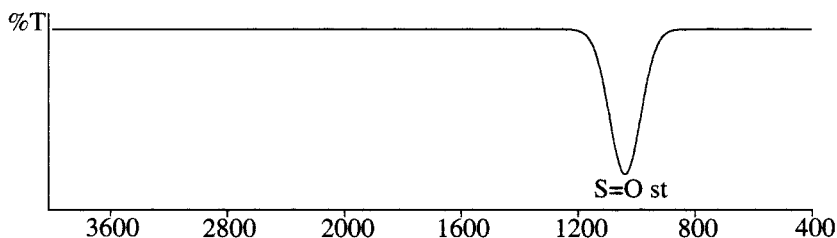
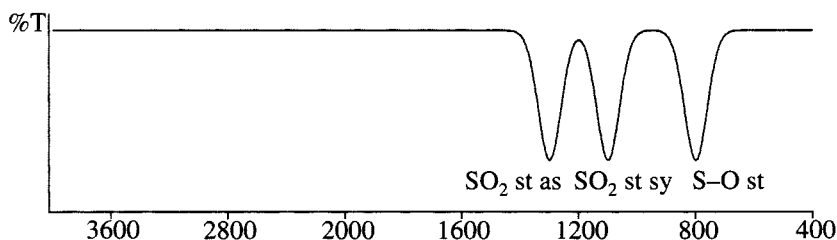
Assignment	Range	Comments
<b>S-H st</b>	2600–2540	Often weak, narrow
<b>S-H <math>\delta</math></b>	915–800	Weak, of no practical significance
<b>C-S st</b>	710–570	Weak, broad, of no practical significance
<b>S-S st</b>	$\approx$ 500	Weak, of no practical significance
<b>Also:</b>	$\approx$ 2880	(S-)CH <sub>3</sub> st as
	$\approx$ 2860	(S-)CH <sub>2</sub> st as
	$\approx$ 1430	(S-)CH <sub>3</sub> $\delta$ as
	1330–1290	(S-)CH <sub>3</sub> $\delta$ sy
	$\approx$ 1425	(S-)CH <sub>2</sub> $\delta$
	815–755	S-F st, strong
	$\approx$ 630	S-N st in S-N=O
	725–550	S-C in S-C $\equiv$ N, often doublet

S

*Examples* ( $\nu$  in  $\text{cm}^{-1}$ )


## 6.10.2

## Sulfoxides and Sulfones

*Sulfoxides**Sulfones**Typical Ranges ( $\nu$  in  $\text{cm}^{-1}$ )*

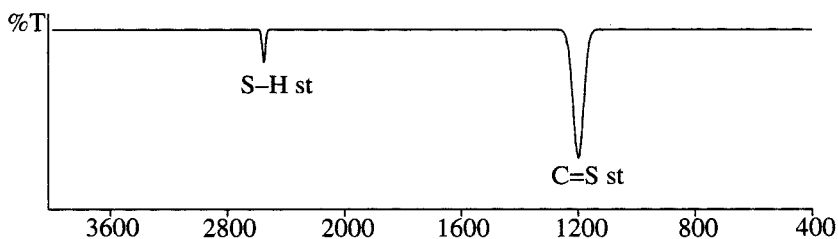
Assignment	Range	Comments
<b>S=O st</b>	1225–980	Strong, sometimes multiple bands
<i>Subranges:</i>		
	1060–1015	R–SO–R
	≈1100	R–SO–OH
		S–O st 870–810
		OH st free ≈3700,
		H-bonded ≈2900, ≈2500
	≈1135	R–SO–OR
	1225–1195	RO–SO–OR
	≈1135	R–SO–Cl
	≈1030, ≈980	R–SO₂⁻
	≈1100, ≈1050	R=SO
		N=SO: ≈1250, ≈1135

S

Assignment	Range	Comments
 st as st sy	1420–1000	Very strong
<i>Subranges:</i>		
	1370–1290, 1170–1110	R–SO <sub>2</sub> –R
	1375–1350, 1185–1165	R–SO <sub>2</sub> –OR
	≈1340, ≈1150	R–SO <sub>2</sub> –SR
	1415–1390, 1200–1185	RO–SO <sub>2</sub> –OR
	1365–1315, 1180–1150	R–SO <sub>2</sub> –N
		N–H st: 3330–3250; N–H δ: ≈1570; S–N st: 910–900
	1410–1375, 1205–1170	R–SO <sub>2</sub> –hal
	1355–1340, 1165–1150	R–SO <sub>2</sub> –OH
		O–H st, H-bonded: ≈2900, ≈2400 hydrated: 2800–1650, broad
	1250–1140, 1070–1030	R–SO <sub>3</sub> <sup>–</sup>
	1315–1220, 1140–1050	RO–SO <sub>3</sub> <sup>–</sup>
S–O st	870–690	Of variable intensity, weak in sulfites

## 6.10.3

## Thiocarbonyl Derivatives

*Typical Ranges ( $\nu$  in  $\text{cm}^{-1}$ )*

Assignment	Range	Comments
<b>C=S st</b>	1275–1030	Strong, narrow
	<i>Subranges:</i>	
	1075–1030	Thioketones
	1210–1080	Thioesters
	≈1215	Dithioacids
	1125–1075	Thioacid fluoride
	1100–1065	Thioacid chloride
<i>Also:</i>	1140–1090	Thioamides and thiolactams
	750–580	P=S st

SH st: ≈2550

SH δ: ≈860

perfluorinated:

1130–1105

perchlorinated:

1100–1075

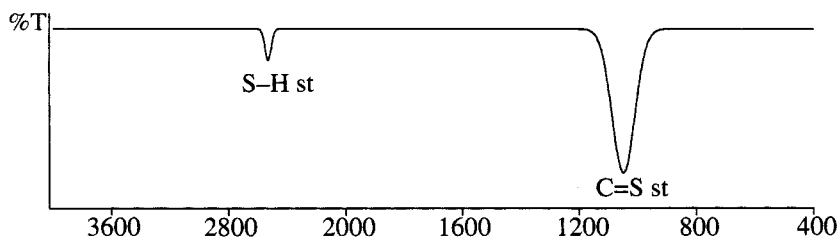
C–N st: 1535–1520

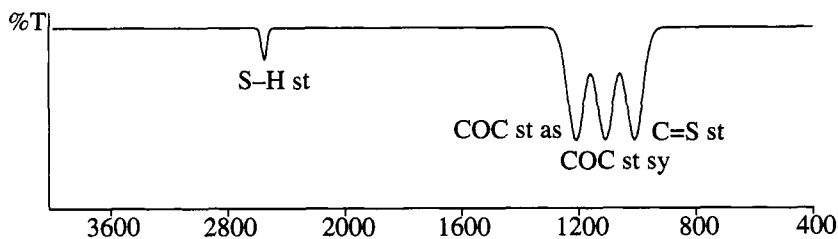
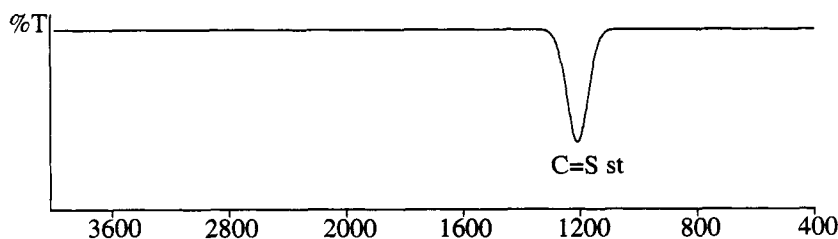
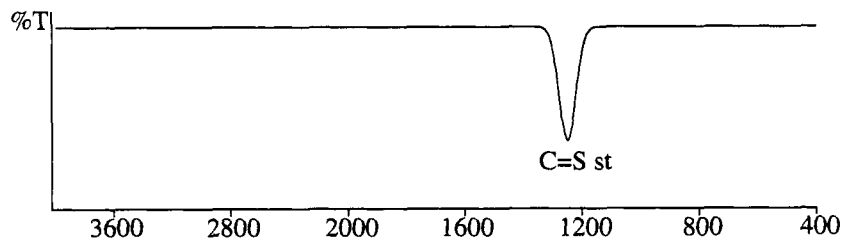
NH δ: 1380–1300

S

## 6.10.4

## Thiocarbonic Acid Derivatives

*Trithiocarbonates*

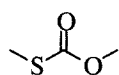
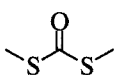
**Xanthates****Thiocarbonates****Thioureas**

S

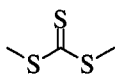
**Typical Ranges ( $\nu$  in  $\text{cm}^{-1}$ )**

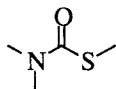
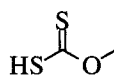
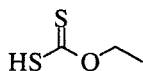
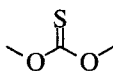
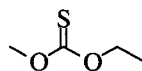
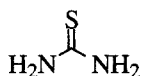
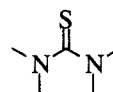
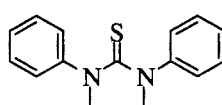
Assignment	Range	Comments	
<b>S-H st</b>	2560–2510	Weak, narrow	trithiocarbonates
	2600–2500	Weak, narrow	xanthates
<b>C=S st</b>	1100–1020	Very strong	trithiocarbonates
	1070–1000	Strong	xanthates
	1250–1180	Strong	thiocarbonates
	1400–1100	Strong	thioureas
<b>COC st as</b>	1260–1140	Strong	xanthates
<b>COC st sy</b>	1150–1090	Strong to medium	xanthates



**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )
 in  $\text{CCl}_4$ :  
1719

 in  $\text{CCl}_4$ :  
1653

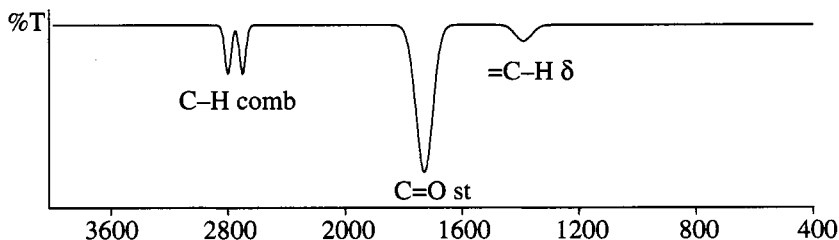
 in  $\text{CCl}_4$ :  
1757

 in  $\text{CCl}_4$ :  
1718  
1677  
1640

 neat:  
1076

 solid:  
1058  
in  $\text{CCl}_4$ :  
1083  
1079

 in  $\text{CCl}_4$ :  
1662

 gas:  
2593  
2548  
neat:  
2470

 in  $\text{CS}_2$ :  
2562  
2522

 solid:  
1212

 solid:  
1234

 solid:  
1400

 solid:  
1130

 solid:  
1131

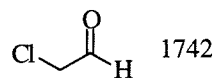
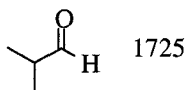
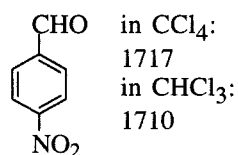
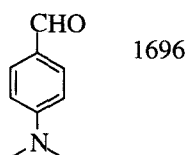
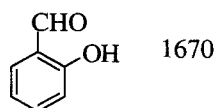
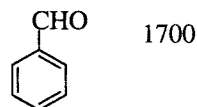
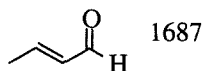
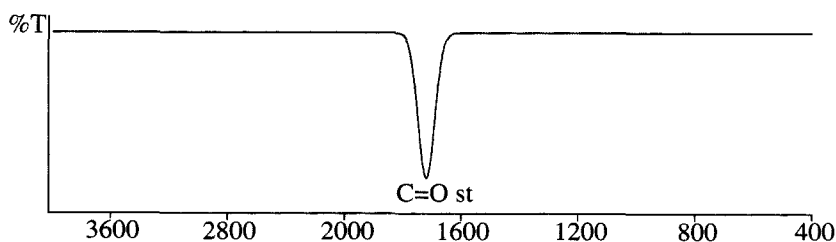
## 6.11 Carbonyl Compounds

### 6.11.1 Aldehydes



#### *Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )*



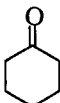
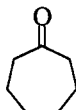
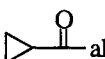
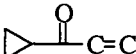
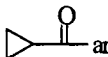
Assignment	Range	Comments
<b>C-H comb</b>	2900-2800	Weak, Fermi resonance with C-H $\delta$ at $\approx$ 1390
	2780-2680	
		For extreme position of C-H $\delta$ only one band
	<i>Subranges:</i>	
	2830-2810, 2720-2690	Aliphatic
	2830-2810, 2750-2720	Aromatic, for <i>o</i> -substitution often higher
	<i>In the same range:</i> cyclohexanes at $\approx$ 2700, weak	
<b>C=O st</b>	1765-1645	Strong
<b>C=X</b>	<i>Subranges:</i>	
	1740-1720	Aliphatic
	1765-1730	$\alpha$ -Halogenated aliphatics
	1710-1685	Aromatic
	1695-1660	$\alpha,\beta$ -Unsaturated aromatic
	1670-1645	With intramolecular H bonds
<b>C-H <math>\delta</math></b>	1390	Weak, of no practical significance

**Examples** ( $\nu$  in  $\text{cm}^{-1}$ ) $\text{CH}_3\text{CHO}$  1748 $\text{CCl}_3\text{CHO}$  1760**6.11.2 Ketones****Typical Ranges** ( $\nu$  in  $\text{cm}^{-1}$ )

Assignment	Range	Comments
<b>C=O st</b>	1775–1650	Strong
	<i>Subranges:</i> $\approx 1715$	Aliphatic, branching at $\alpha$ -position causes shift to lower frequencies:
	$\approx 1775$ –1705	Cyclic, $\nu$ decreases with increasing ring size





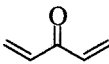
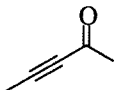
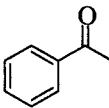
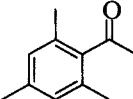
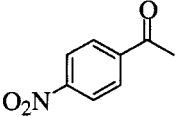
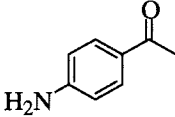
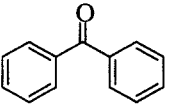
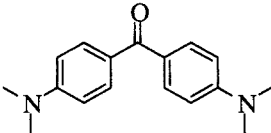
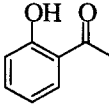

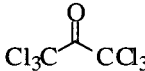
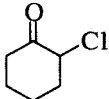
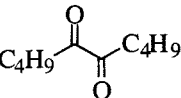


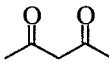
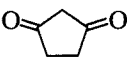
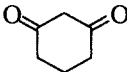
[contd.]

**C=X**

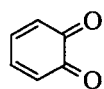
Assignment	Range	Comments																
		 $\approx 1775$  $\approx 1750$																
		 $\approx 1715$  $\approx 1705$																
Conjugated:	$\approx 1675$	$\alpha, \beta$ -Unsaturated, often 2 bands (rotational isomers)																
	1650–1600	C=C st																
	$\approx 1695$	 al																
	$\approx 1665$	$\alpha, \beta; \gamma, \delta$ -Unsaturated; $\alpha, \beta; \alpha', \beta'$ -unsaturated																
	$\approx 1670$	 C=C																
	$\approx 1690$	Aryl ketones																
	$\approx 1675$	 ar																
	$\approx 1665$	Diaryl ketones, with N or O in <i>p</i> -position: down to $\approx 1600$																
$\alpha$ -Halogenated ketones:	Shifted toward higher wavenumbers depending on dihedral angle $\phi$ between C=O and C-hal; largest effect for $\phi = 0^\circ$ , no effect for $\phi = 90^\circ$																	
	Maximal shifts:	<table><tr><td><math>\alpha</math>-chloro</td><td><math>\approx 25</math></td><td><math>\alpha</math>-bromo</td><td><math>\approx 20</math></td></tr><tr><td><math>\alpha, \alpha</math>-dichloro</td><td><math>\approx 45</math></td><td><math>\alpha</math>-iodo</td><td><math>\approx 0</math></td></tr><tr><td><math>\alpha, \alpha'</math>-dichloro</td><td><math>\approx 45</math></td><td><math>\alpha, \alpha</math>-difluoro</td><td><math>\approx 60</math></td></tr><tr><td></td><td></td><td>perfluoro</td><td><math>\approx 90</math></td></tr></table>	$\alpha$ -chloro	$\approx 25$	$\alpha$ -bromo	$\approx 20$	$\alpha, \alpha$ -dichloro	$\approx 45$	$\alpha$ -iodo	$\approx 0$	$\alpha, \alpha'$ -dichloro	$\approx 45$	$\alpha, \alpha$ -difluoro	$\approx 60$			perfluoro	$\approx 90$
$\alpha$ -chloro	$\approx 25$	$\alpha$ -bromo	$\approx 20$															
$\alpha, \alpha$ -dichloro	$\approx 45$	$\alpha$ -iodo	$\approx 0$															
$\alpha, \alpha'$ -dichloro	$\approx 45$	$\alpha, \alpha$ -difluoro	$\approx 60$															
		perfluoro	$\approx 90$															
$\alpha$ -Diketones:	$\approx 1720$	Aliphatic																
	$\approx 1775, \approx 1760$	Aliphatic 5-ring																
	$\approx 1760$	Aliphatic 6-ring																
	$\approx 1730$																	
	$\approx 1675$	Aliphatic enolized, C=C st: $\approx 1650$																
	$\approx 1680$	Aromatic																
	$\approx 1675$	<i>o</i> -Quinones, with <i>peri</i> -OH: $\approx 1675, \approx 1630$																
$\beta$ -diketones:	$\approx 1720$	Keto form, sometimes doublet																
	$\approx 1650$	Enol form																
	$\approx 1615$	Enol with intramolecular H bonds, C=C st: $\approx 1600$ strong																

Assignment	Range	Comments
$\gamma$ -diketones:		As monoketones
	$\approx 1675$	<i>p</i> -Quinones, with <i>peri</i> -OH: $\approx 1675$ , $\approx 1630$ ; C=C st: $\approx 1600$
C=C=O st as	2155–2130	Very strong

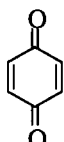
**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )

 1691	 1697	 $\rightleftharpoons$  <i>s-trans</i> 1690 <i>s-cis</i> 1707
 1672 1660	 1678 (2222)	 1692
 1701	 1702	 1676
 1664	 1639	 1648
 1752 1726 (rotamers)	 1780 1751	 1722
 1710	 1700 1655	 1735
 1724 (keto form) 1608 (enol form)	 1755 1725 1635 1590	 1630 1607

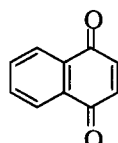
C = X



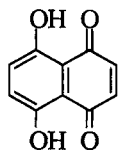
1669



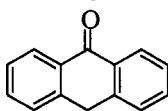
1669



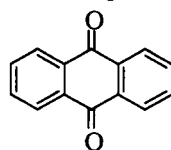
1675



1623



1662

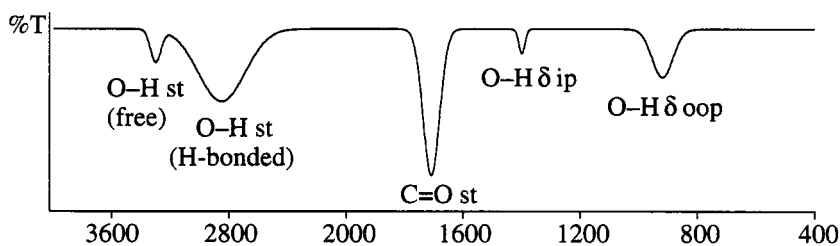


1678

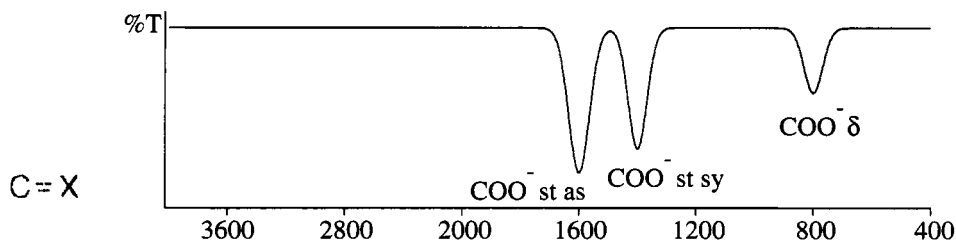
### 6.11.3

### Carboxylic Acids

#### Carboxylic Acids



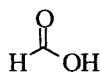
#### Carboxylate Anions



*Typical Ranges ( $\nu$  in  $\text{cm}^{-1}$ )*

Assignment	Range	Comments
<b>COO-H st</b>	3550–2500	intensity variable
	<i>Subranges:</i>	
	3550–3500	Free, sharp, only in highly diluted solutions
	3300–2500	H-bonded, broad, often more than one band
	<i>In the same range also OH st, NH st, CH st, SiH st, SH st, PH st</i>	
<b>C=O st</b>	1800–1650	Strong
	1800–1740	Free (also in dicarboxylic acids)
	1740–1650	H-bonded (dimer, also in dicarboxylic acids)
	<i>Subranges for H-bonded C=O:</i>	
	1725–1700	al-COOH
	1715–1690	C=C-COOH
	1700–1680	ar-COOH
	1740–1720	hal-C-COOH
	1670–1650	Intramolecular H bond
<b>OC-OH st,</b>	1440–1210	Of no practical significance
<b>C-OH <math>\delta</math></b>		
<b>OC-OH <math>\delta</math> oop</b>	960–880	Medium, generally broad (only in dimers), in the same range: =CH $\delta$ , ar CH $\delta$ , NH $\delta$
<b>(COO)<sup>-</sup> st as</b>	1610–1550	Very strong; in $\alpha$ -halogen carboxylates near the higher value, with more than one $\alpha$ -hal beyond the normal range; in polypeptides at $\approx 1575$
<b>(COO)<sup>-</sup> st sy</b>	1450–1400	Strong, of no practical significance, in polypeptides at $\approx 1470$
<b>(COO)<sup>-</sup> <math>\delta</math></b>	$\approx 775$	Formates, weak
	$\approx 925$	Acetates
	$\approx 680$	Benzoates
	$\approx 600$	CF <sub>3</sub> COO <sup>-</sup>

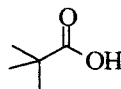
C=X

*Examples ( $\nu$  in  $\text{cm}^{-1}$ )*

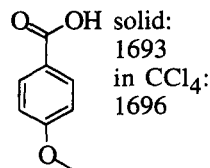
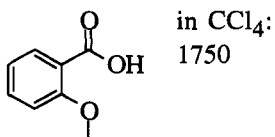
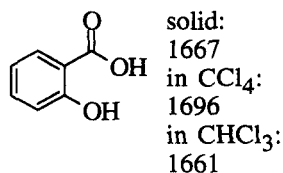
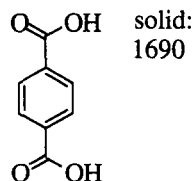
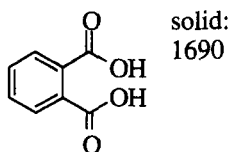
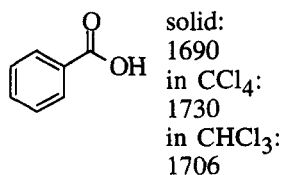
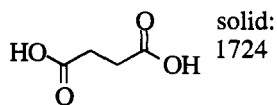
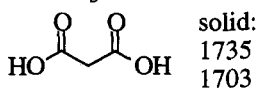
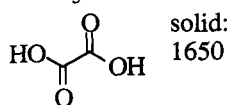
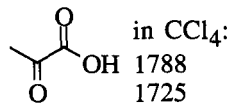
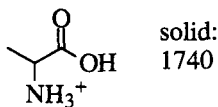
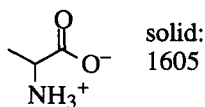
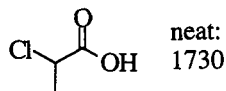
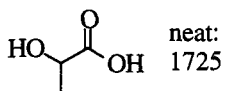
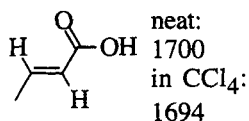
neat:  
1727  
in CCl<sub>4</sub>:  
1756  
1724



neat:  
1759  
1718  
in CCl<sub>4</sub>:  
1768  
1717

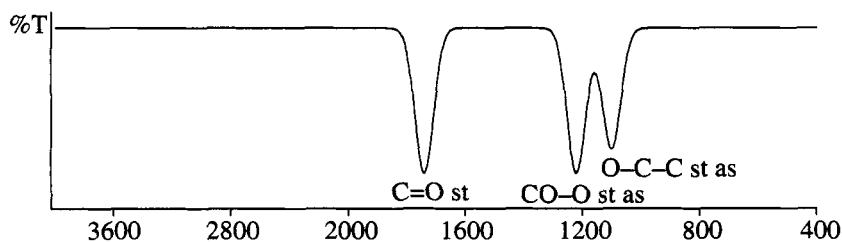


in CCl<sub>4</sub>:  
1704  
solid:  
1686











## 6.11.4

## Esters and Lactones

 $\text{C}=\text{X}$ 

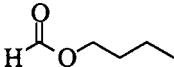
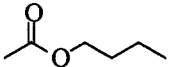
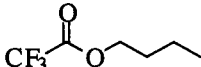
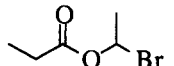
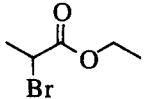
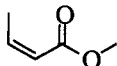
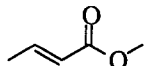
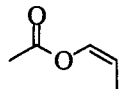
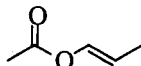
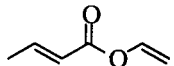
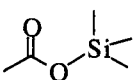
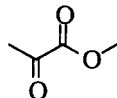
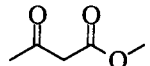
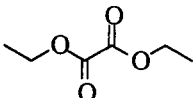
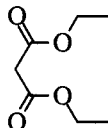
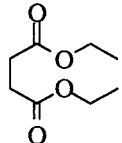
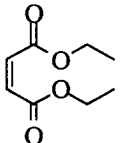
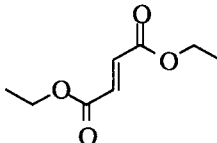
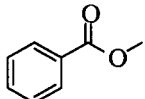
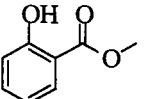
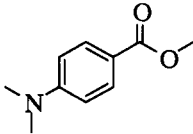
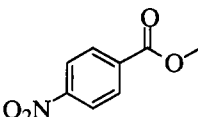
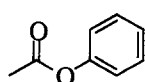
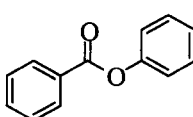
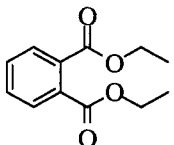


*Typical Ranges* ( $\nu$  in  $\text{cm}^{-1}$ )

Assignment	Range	Comments
<b>C=O st</b>	1790–1650	Strong
	<i>Subranges:</i>	
	1750–1735	Aliphatic esters
<i>Conjugated esters:</i>	1730–1710	$\alpha,\beta$ -Unsaturated esters
	1730–1715	Aromatic esters
	1690–1670	With intramolecular H bonds
	1790–1740	$\alpha$ -Halogenated esters
	$\approx 1760$	Vinyl esters, C=C st: 1690–1650, strong
	$\approx 1760$	Phenol esters
	$\approx 1735$	Phenol esters of an aromatic acid
<i>Diesters:</i>		As the corresponding monoesters
<i>Keto esters:</i>	1755–1725	$\alpha$ -Keto esters, generally one band
	$\approx 1750$ (ketone)	$\beta$ -Ketoesters, keto form
	$\approx 1735$ (ester)	
	$\approx 1650$	$\beta$ -Ketoesters, enol form, C=C st: $\approx 1630$ , strong
	$\approx 1740, \approx 1715$	$\gamma$ -Ketoesters, pseudoesters: $\approx 1770$
<i>Lactones:</i>	 $\approx 1840$  $\approx 1770$  $\approx 1800$	
	 $\approx 1750$ (additional band at $\approx 1780$ if $\alpha$ -position free)  $\approx 1735$	
	 $\approx 1760$  $\approx 1720$  $\approx 1730$ (often doublet)	
<b>C–O st</b>	1330–1050	2 bands: st as, very strong and at higher frequency; st sy, strong, at lower frequency
<b>C–O st as:</b>	<i>Subranges:</i>	
	$\approx 1185$	Formates, propionates, higher aliphatic esters
	$\approx 1240$	Acetates
	$\approx 1210$	Vinyl esters, phenol esters
	$\approx 1180$	$\gamma$ -Lactones, $\delta$ -lactones
	$\approx 1165$	Methyl esters of aliphatic acids
	<i>In the same range:</i> Strong bands for	
	C–F st, C–N st, N–O st, P–O st, C=S st, S=O st, P=O st, Si–O st, Si–H $\delta$	

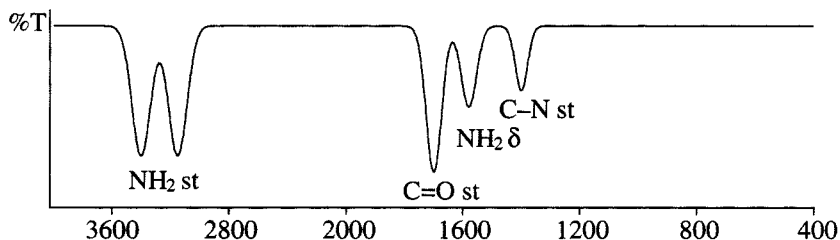
C = X

**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )

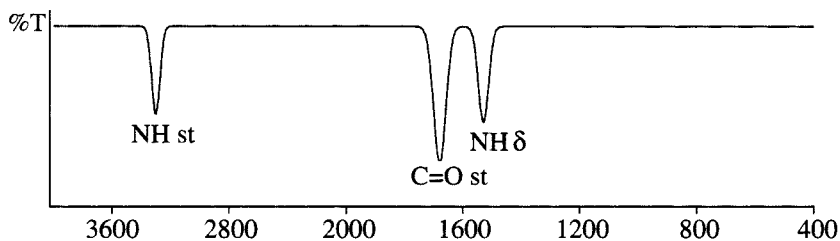
	1730		1743		1787
	1747		1743		1724
	1726		1758 (1690)		1752 (1675)
	1730 (1658) (1638)		1725		1725
	ester: 1704 ketone: 1690 enol: 1645		1774 1754		1760 1742
	1740		1734		1727
	1727		1684		1715
<b>C=X</b>					
	1737		1766		1743
	1746				

### 6.11.5 Amides and Lactams

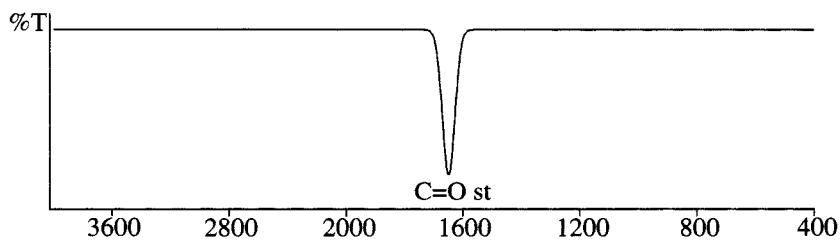
#### Primary Amides



#### Secondary Amides



#### Tertiary Amides

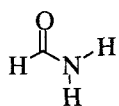


C = X

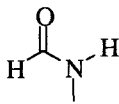
#### Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )

Assignment	Range	Comments
<b>N-H st</b>	3500–3100	Medium, in primary amides two bands, in proteins multiplet
<i>Subranges:</i>		
	3500–3400	Free
	3350–3100	H-bonded
	$\approx 3350, \approx 3180$ In primary amides generally two bands	

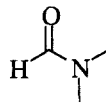
Assignment	Range	Comments
	≈3200, ≈3100	In lactams generally two bands
	≈3200	Monohydrazides
	≈3100	Dihydrazides
	≈3250	Imides
	<i>In the same range:</i> OH st, ≡CH st (≈3300, sharp), H <sub>2</sub> O	
<b>C=O st (amide I)</b>	1740–1630	Generally strong
	<i>Subranges:</i>	
	≈1690	NH <sub>2</sub> C=O free amides, H-bonded: ≈1650
	≈1685	NHC=O free amides, H-bonded: ≈1660
	≈1650	NC=O free amides, H-bonded: ≈1650
	≈1745	4-Ring lactams
	≈1700	5-Ring lactams
	≈1650	6-, 7-Ring lactams
	≈1670	Monohydrazides
	≈1600	Dihydrazides
	1740–1670	Imides
	≈1750, 1700	5-Ring imides, 2 bands
	1655–1630	Polypeptides
	≈1690	Isocyanurates, with aromatic substitution at ≈1770
	≈1720	
	1755 sh	Trifluoroacetamides
<b>NH δ and N–C=O st sy (amide II)</b>	1630–1510	Generally strong, absent in lactams
	<i>Subranges:</i>	
	≈1610	NH <sub>2</sub> C=O free, H-bonded: ≈1630
	≈1530	NHC=O, H-bonded: ≈1540
	1560–1510	Polypeptides
	≈1555	Trifluoroacetamides
<b>C=N st (?)</b>	≈1400	NH <sub>2</sub> C=O
	≈1250	NHC=O
	≈1330	Lactams
<b>NH δ ip</b>	≈1150	NH <sub>2</sub> C=O
	≈1465	Lactams
<b>NH δ oop</b>	750–600	NH <sub>2</sub> C=O
	≈700	NHC=O
	≈800	Lactams

*Examples ( $\nu$  in  $\text{cm}^{-1}$ )*

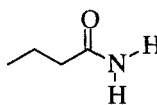
neat:  
1672  
in  $\text{CHCl}_3$ :  
1709



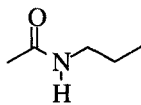
neat:  
1672



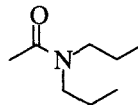
neat:  
1670  
in  $\text{CHCl}_3$ :  
1673



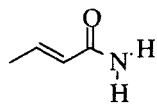
solid:  
1631  
in  $\text{CHCl}_3$ :  
1679



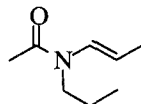
in  $\text{CCl}_4$ :  
1690



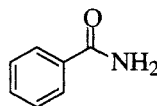
in  $\text{CCl}_4$ :  
1647



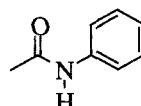
solid:  
1677



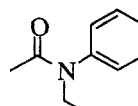
in  $\text{CS}_2$ :  
1675  
1650



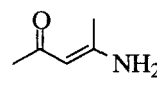
solid:  
1656  
in  $\text{CHCl}_3$ :  
1678



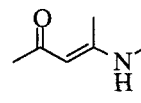
solid:  
1658  
in  $\text{CHCl}_3$ :  
1691  
in  $\text{CCl}_4$ :  
1705



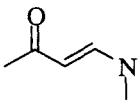
in  $\text{CCl}_4$ :  
1667



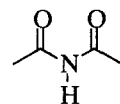
neat:  
1700  
1625  
1540



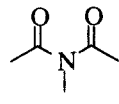
solid:  
1628  
1595



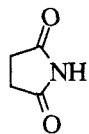
solid:  
1631  
1584



solid:  
1734  
1505

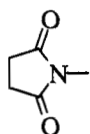


solid:  
1736  
1706  
1689

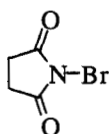


solid:  
1771  
1698  
in  $\text{CCl}_4$ :  
1753  
1727

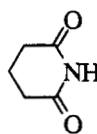
C=X



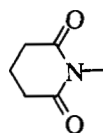
solid:  
1760  
1690  
in  $\text{CCl}_4$ :  
1721  
1705



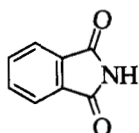
in  $\text{CHCl}_3$ :  
1783  
1733



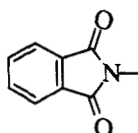
in  $\text{CCl}_4$ :  
1742  
1730  
1718



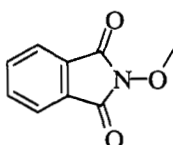
solid:  
1718  
1670  
in  $\text{CCl}_4$ :  
1729,  
1686



solid:  
1774  
1749  
1724  
in  $\text{CHCl}_3$ :  
1778  
1735



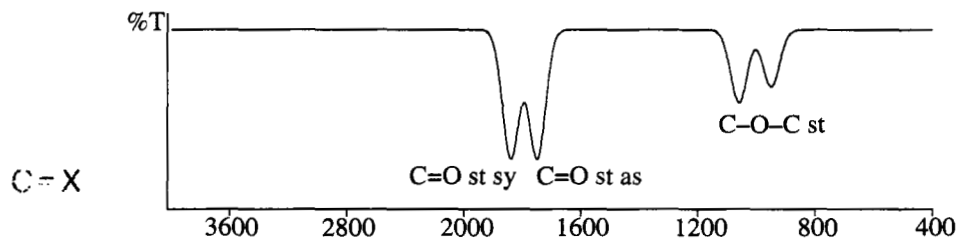
in  $\text{CHCl}_3$   
1772  
1712



solid:  
1790  
1735

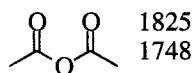
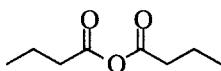
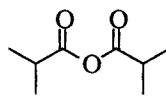
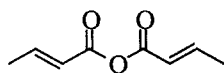
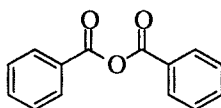
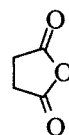
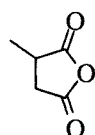
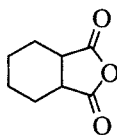
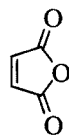
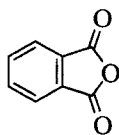
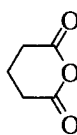
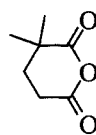
### 6.11.6

#### Acid Anhydrides



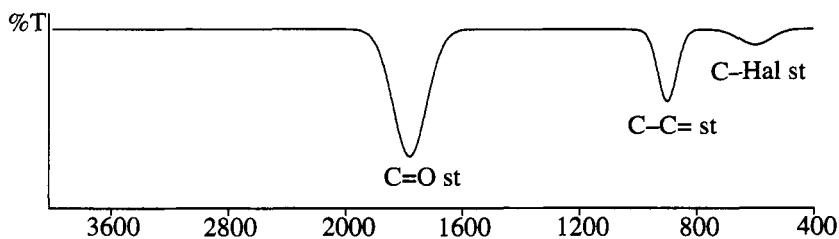
*Typical Ranges ( $\nu$  in  $\text{cm}^{-1}$ )*

Assignment	Range	Comments
<b>C=O st sy</b>	1870–1770	Strong
<b>C=O st as</b>	1800–1720	Strong
<i>Subranges:</i>		
	$\approx 1820, \approx 1760$	Linear anhydrides, higher band stronger
	$\approx 1850, \approx 1775$	5-Ring, lower band stronger
	$\approx 1800, \approx 1760$	6-Ring, lower band stronger
<b>C–O–C st</b>	1300–900	Strong, several bands
	$\approx 1040$	Linear anhydrides
	$\approx 920$	Cyclic anhydrides

*Examples ( $\nu$  in  $\text{cm}^{-1}$ )*1825  
17481810  
1740  
1045  
10401803  
17431780  
17251790  
1727  
1035  
1015  
9951865  
1782  
9201859  
17891845  
17801850  
1800  
9001840  
1810  
1760  
9121802  
17611802  
1761

C=X

### 6.11.7 Acid Halides



#### *Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )*

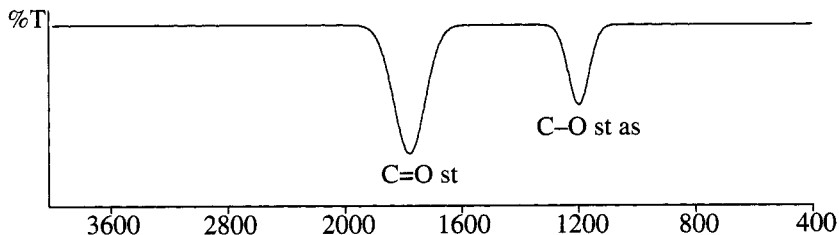
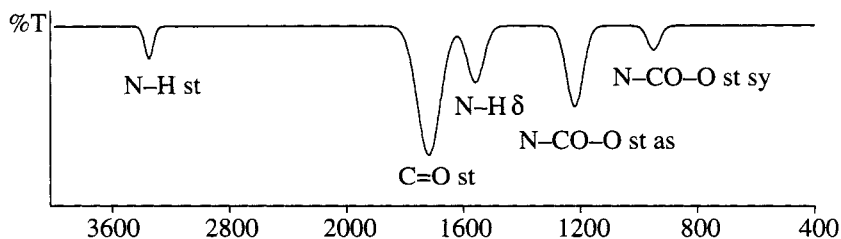
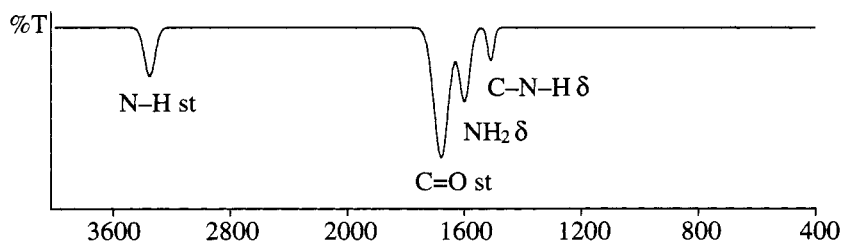
Assignment	Range	Comments
<b>C=O st</b>	1820–1750	chlorides, strong, of narrow or medium width, for bromides and iodides at lower frequency
	1900–1870	fluorides, strong, of narrow or medium width, additional band at $\approx 1725$ in aromatic acid chlorides and bromides
<b>C-CO st</b>	1000–800	1000–900 al, assignment uncertain
		900–800 ar, assignment uncertain
<b>C-hal st</b>	1200–500	1200–800 F
		750–550 Cl
		700–500 Br
		600–500 I

C = X



## 6.11.8

## Carbonyl Acid Derivatives

*Carbonyl Acid Derivatives**Carbamates**Ureas*

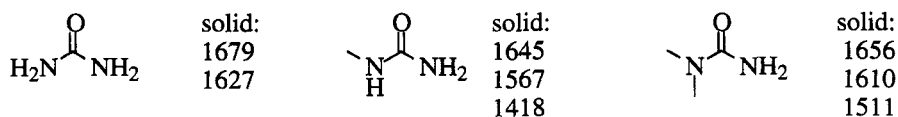
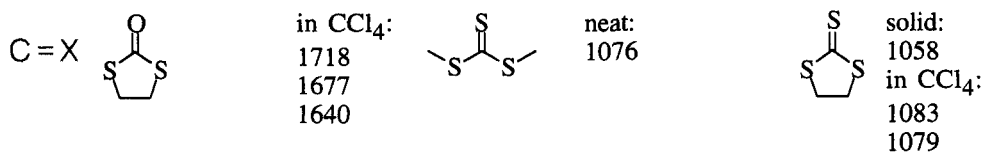
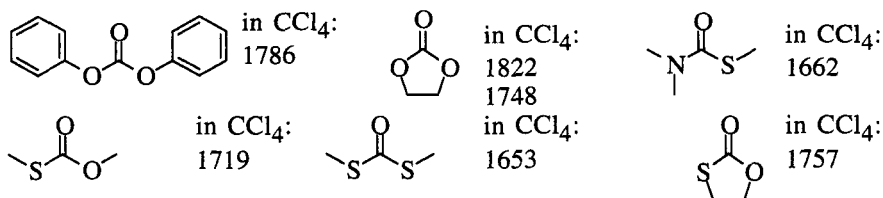
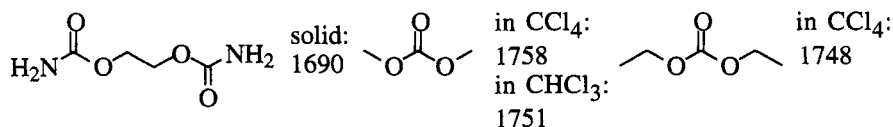
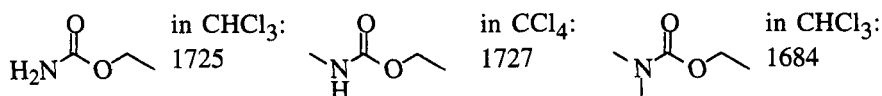
C = X

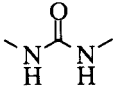
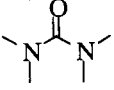
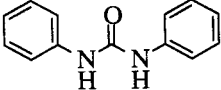
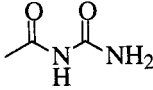
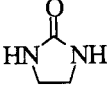
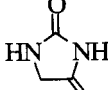
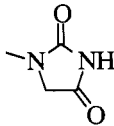
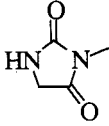
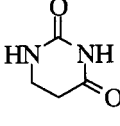
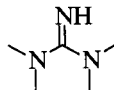
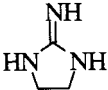
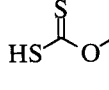
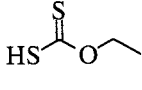
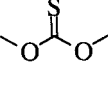
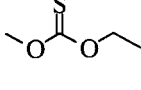
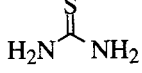
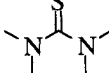
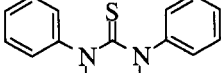
*Typical Ranges (ν in cm<sup>-1</sup>)*

Assignment	Range	Comments
<b>C=O st</b>	1820–1740	Strong carbonyl acid derivatives
	1750–1680	Strong carbamates
	1690–1620	Strong ureas
<b>C–O st as</b>	1260–1150	Strong carbonyl acid derivatives

Assignment	Range	Comments
<b>N-H st</b>	3500-3250	Medium, two bands for $\text{NH}_2$ , one for NH
	3500-3200	Medium, two bands for $\text{NH}_2$
<b>N-H <math>\delta</math></b>	1650-1500	Medium
<b><math>\text{NH}_2</math> <math>\delta</math></b>	1650-1600	Medium
<b>N-CO-O st as</b>	1270-1210	Medium
<b>N-CO-O st sy</b>	1050-850	Weak
<b>C-N-H <math>\delta</math></b>	1600-1500	Weak

**Examples** ( $\nu$  in  $\text{cm}^{-1}$ )

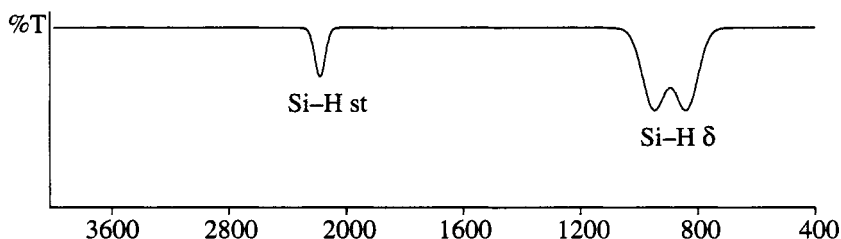


	solid: 1622 1580 1530 in CHCl <sub>3</sub> : 1663 1548		solid: 1645 1560 1497 CHCl <sub>3</sub> : 1675		solid: 1650
	solid: 1667 1634		in CCl <sub>4</sub> : 1735 1718		solid: 1776 1697
	solid: 1712 1676		solid: 1748 1706		solid: 1767 1695
	neat: 1600		solid: 1767 1681 1621		gas: 2593 2548 neat: 2470
	in CS <sub>2</sub> : 2562 2522		solid: 1212		solid: 1234
	solid: 1400		solid: 1130		solid: 1131

C=X

## 6.12 Miscellaneous Compounds

### 6.12.1 Silicon Compounds



#### *Typical Ranges* ( $\nu$ in $\text{cm}^{-1}$ )

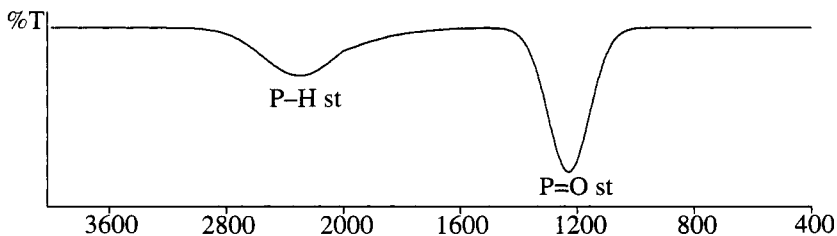
Assignment	Range	Comments
<b>Si-H st</b>	2250–2090	Medium
	<i>Subranges:</i>	
	2160–2090	$\text{R}_3\text{Si-H}$ ; also for R as H, for $\text{SiH}_3$ 2 bands
	$\approx 2250$	hal-Si-H
	2220–2120	(Si-O)Si-H
<b>Si-H <math>\delta</math></b>	1010–700	Strong, broad, generally 2 bands
<b>(Si-)CH<sub>3</sub> <math>\delta</math> as</b>	$\approx 1410$	Weak
<b>(Si-)CH<sub>3</sub> <math>\delta</math> sy</b>	1275–1260	Very strong, sharp, typical for $\text{SiCH}_3$ , not split for $\text{Si}(\text{CH}_3)_2$
<b>(Si-)CH<sub>3</sub> <math>\gamma</math></b>	860–760	
	$\approx 765$	$\text{SiCH}_3$
	$\approx 855, \approx 800$	$\text{Si}(\text{CH}_3)_2$
	$\approx 840, \approx 765$	$\text{Si}(\text{CH}_3)_3$
Misc. <b>Si-O st</b>	1110–1000, 900– <600	
	1110–1000, 850–800	Si-O-C
	1090–1030, < 650	Si-O-Si
	900–800	Si-OH
	3700–3200	Si-OH st
	$\approx 1030$	Si-OH $\delta$

Assignment	Range	Comments
<b>Si-C st</b>	850–650	
<b>Si-N st</b>	1250–830	
	<i>Subranges:</i>	
	950–830	Si–N–Si
	≈3400	Si <sub>2</sub> NH st
	950–830	N–Si–N
	1250–1100	Si–NH <sub>2</sub>
	≈3570, ≈3390	SiN–H <sub>2</sub> st
	≈1540	Si–NH <sub>2</sub> δ
<b>Si-F st</b>	980–820	
	<i>Subranges:</i>	
	920–820	Si–F
	945–870	Si–F <sub>2</sub> , 2 bands
	980–860	Si–F <sub>3</sub> , 2 bands
<b>Si-Cl st</b>	< 625	

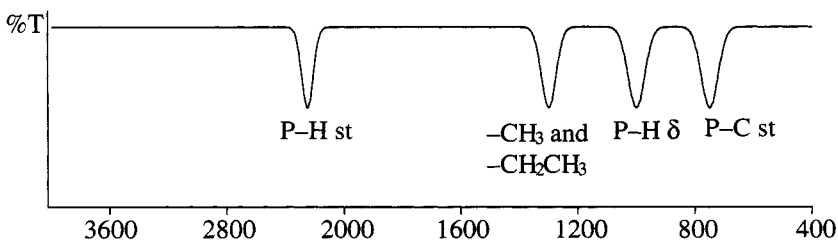
### 6.12.2

### Phosphorus Compounds

#### Phosphorous Compounds



#### Phosphines



Misc.

**Typical Ranges** ( $\nu$  in  $\text{cm}^{-1}$ )

Assignment	Range	Comments
<b>P-H st</b>	2440–2275	Weak to medium, generally one band, in $\text{R}_3\text{PH}^+$ very broad
<b>PO-H st</b>	2700–2650	Weak, very broad
<b>POH comb</b>	2300–2250	Weak, very broad
	1740–1600	Additional band in $\text{O}=\text{P}-\text{OH}$ (dimer?)
<b>P-O st</b>	1260–855	
	<i>Subranges:</i>	
	1050–970, 830–740	P–O–C al st; strong and often weak for upper and lower band, respectively
	1260–1160	P–O–C ar st
	995–915	P(V)
	875–855	P(III)
	1100–940	P–OH st, broad, for $\text{P}(\text{OH})_2$ often two bands
	980–900	P–O–P st
<b>P=O st</b>	1300–960	Strong
	<i>Subranges:</i>	
	1190–1150	$\text{R}_3\text{P}=\text{O}$ , also for R: H
	1265–1200	$\text{R}_2(\text{R}'\text{O})\text{P}=\text{O}$ , also for R: H
	1280–1240	$\text{R}(\text{R}'\text{O})_2\text{P}=\text{O}$ , also for R: H
	1300–1260	$(\text{RO})_3\text{P}=\text{O}$
	1220–1150	$\text{R}(\text{HO})_2\text{P}=\text{O}$
	1250–990	$\text{R}(\text{HO})\text{PO}_2^-$ , more than one band
	1125–970, 1000–960	$\text{RPO}_3^{2-}$
	1205–1090	$\text{R}_2(\text{HO})\text{P}=\text{O}$
	1200–1090, 1090–995	$\text{R}_2\text{PO}_2^-$
	$\approx 1250$	$\text{RO}(\text{HO})_2\text{P}=\text{O}$
	1230–1210, 1030–1020	$\text{RO}(\text{HO})\text{PO}_2^-$
Misc.	1140–1050, 1010–970	$\text{ROPO}_3^{2-}$
	1250–1210	$(\text{RO})_2(\text{HO})\text{P}=\text{O}$
	1285–1120, 1120–1050	$(\text{RO})_2\text{PO}_2^-$
	1220–1170	$\text{R}(\text{RO})(\text{HO})\text{P}=\text{O}$
	1245–1150, 1110–1050	$\text{R}(\text{RO})\text{PO}_2^-$

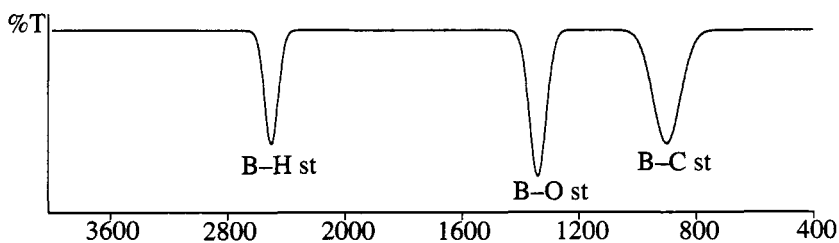
Assignment	Range	Comments
	1240–1205	$\begin{array}{c} \text{R} \quad \text{O} \quad \text{O} \quad \text{R} \\ \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \text{R}-\text{P}-\text{O}-\text{P}-\text{R} \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \end{array}$
	1310–1260	$\begin{array}{c} \text{RO} \quad \text{O} \quad \text{O} \quad \text{OR} \\ \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \text{RO}-\text{P}-\text{O}-\text{P}-\text{OR} \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \end{array}$
	$\approx 1195$	$\begin{array}{c} \text{HO} \quad \text{O} \quad \text{O} \quad \text{OH} \\ \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \text{R}-\text{P}-\text{O}-\text{P}-\text{OR} \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \end{array}$
	$\approx 1275$	$\begin{array}{c} \text{RO} \quad \text{O} \quad \text{O} \quad \text{OR} \\ \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \text{R}_2\text{N}-\text{P}-\text{O}-\text{P}-\text{NR}_2 \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \end{array}$
	1265–1250	$\begin{array}{c} \text{R} \quad \text{O} \quad \text{O} \quad \text{R} \\ \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \text{RO}-\text{P}-\text{O}-\text{P}-\text{OR} \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \end{array}$
	$\approx 1300, \approx 1240$	$\begin{array}{c} \text{RO} \quad \text{O} \quad \text{O} \quad \text{NR}_2 \\ \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \text{RO}-\text{P}-\text{O}-\text{P}-\text{NR}_2 \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \end{array}$
	$\approx 1250$	$\begin{array}{c} \text{RO} \quad \text{O} \quad \text{O} \quad \text{OR} \\ \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \text{HO}-\text{P}-\text{O}-\text{P}-\text{OH} \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \end{array}$
	$\approx 1235$	$\begin{array}{c} \text{R}_2\text{N} \quad \text{O} \quad \text{O} \quad \text{NR}_2 \\ \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \text{R}_2\text{N}-\text{P}-\text{O}-\text{P}-\text{NR}_2 \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \end{array}$
	1265–1240	$\text{R}_2(\text{X})\text{P}=\text{O}$ , X: F, Cl, Br
	1365–1260	$\text{R}(\text{X})_2\text{P}=\text{O}$ , X: F, Cl, Br
	1330–1280	$(\text{RO})_2(\text{X})\text{P}=\text{O}$ , X: F, Cl, Br
	1365–1260	$\text{RO}(\text{X})_2\text{P}=\text{O}$ , X: F, Cl, Br
<b>P=N</b>	1500–1170	
<b>P–OH <math>\delta</math></b>	$\approx 1280$	Weak, of no practical significance
<b>P–C st</b>	800–700	Intensity varies widely, of no practical significance
<b>P–H <math>\delta</math></b>	1090–910	Strong, for $(\text{RO})_2\text{HP}=\text{O}$ very strong
<b>P–N–C st</b>	1110–930, 770–680	
<b>P=N–al st</b>	1500–1230	
<b>P=N–ar st</b>	1390–1300	
<b>P=N–C=O st</b>	1370–1310	
<b>P=N–PR<sub>2</sub> st</b>	1295–1170	
<b>P=S st</b>	750–580	Intensity varies widely
<b>P–S st</b>	<600	
<b>(P–)CH<sub>3</sub> <math>\delta</math> sy</b>	1310–1280	

Misc.

Assignment	Range	Comments
<b>P-F st</b>	905–760	
<b>PF<sub>2</sub></b>	1110–800	More than one band
<b>P-Cl st</b>	<600	

### 6.12.3

### Boron Compounds



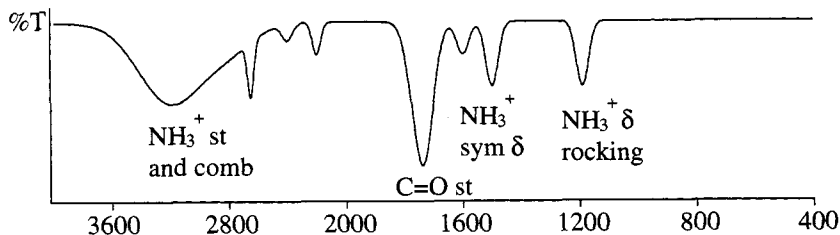
### Typical Ranges ( $\nu$ in $\text{cm}^{-1}$ )

Assignment	Range	Comments
<b>B-H st</b>	2640–2200	Strong
	2200–1540	B–H...B, more than one band
<b>B-O st</b>	1380–1310	Very strong
	≈1500	Haloboroxines
<b>BO-H st</b>	3300–3200	Very broad
<b>B-N st</b>	1550–1330	Very strong
<b>B-C st</b>	1240–620	Strong, 2 bands if substitution highly asymmetric
<b>B-F st</b>	1500–800	
<b>B-Cl st</b>	1100–650	

Misc.



## 6.13 Amino Acids



### *Typical Ranges* ( $\nu$ in $\text{cm}^{-1}$ )

Assignment	Range	Comments
<b>N-H st</b>	3400–2000	Generally strong, broad, very structured
<b>O-H st</b>		
	<i>Subranges:</i>	
	3100–2000	Zwitterions, distinct side band at 2200–2000
	3350–2000	Hydrochlorides
	3400–3200	$\text{Na}^+$ salts
<b><math>\text{NH}_3^+</math> <math>\delta</math> as</b>	1660–1590	Weak, for hydrochlorides near the lower limit
<b><math>\text{NH}_3^+</math> <math>\delta</math> sy</b>	1550–1480	Medium
<b><math>\text{COO}^-</math> st as</b>	1760–1595	Strong
	<i>Subranges:</i>	
	$\approx 1595$	Zwitterions
	1755–1700	Hydrochlorides, in $\alpha$ -amino acids: 1760–1730
	$\approx 1595$	$\text{Na}^+$ salts

## 6.14

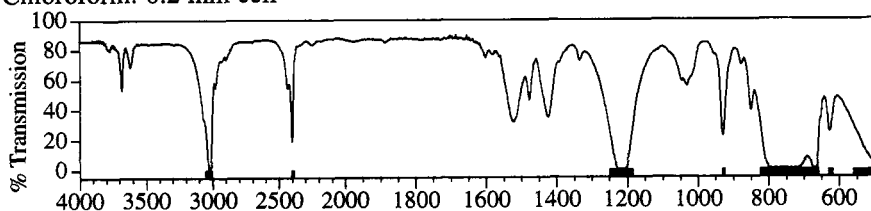
### Solvents, Suspension Media, and Interferences

#### 6.14.1

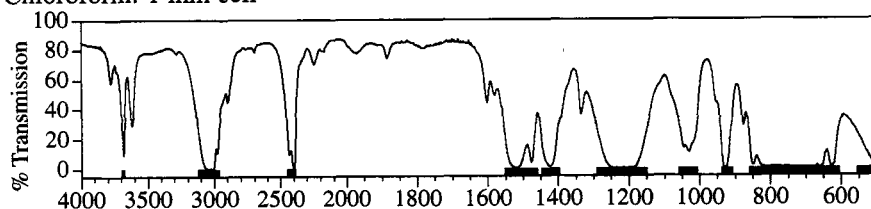
##### Infrared Spectra of Common Solvents

The low transmission in regions where the solvent absorbs may lead to artifacts. For the interpretation of spectra, these regions should be disregarded. In the following, they are indicated by bars.

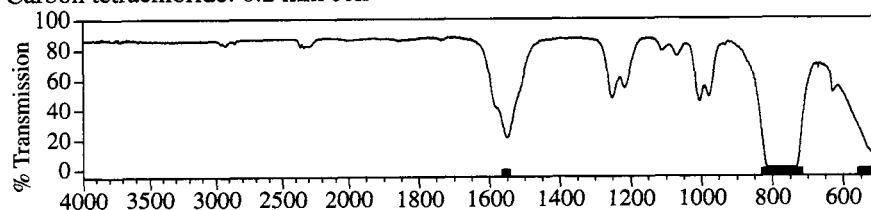
Chloroform: 0.2 mm cell



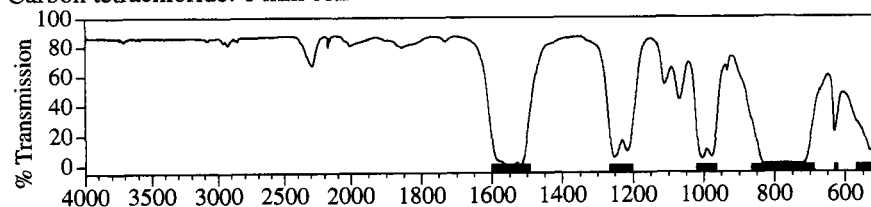
Chloroform: 1 mm cell



Carbon tetrachloride: 0.2 mm cell

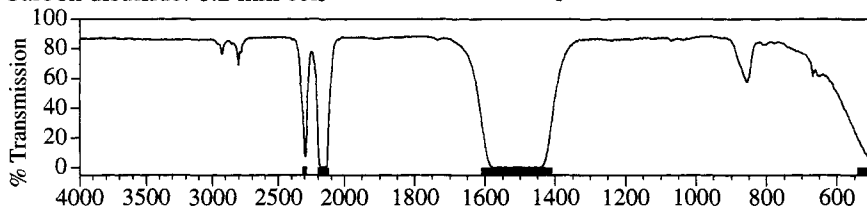


Carbon tetrachloride: 1 mm cell

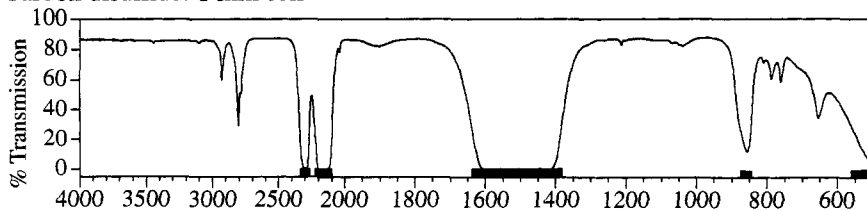


Solvents

Carbon disulfide: 0.2 mm cell



Carbon disulfide: 1 mm cell

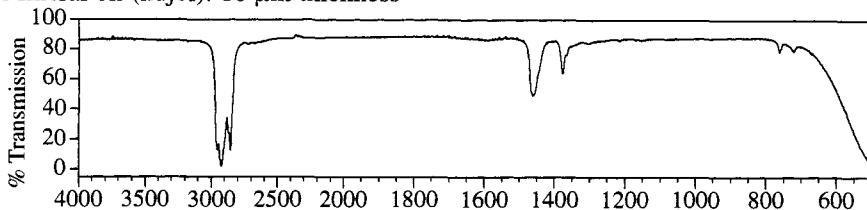


### 6.14.2

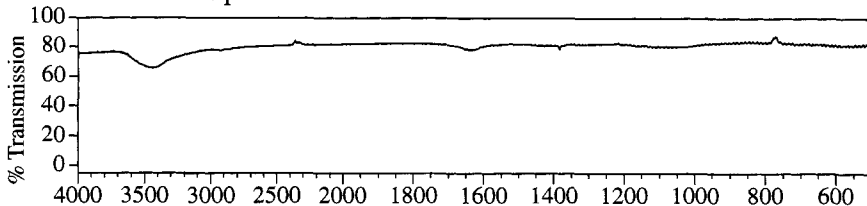
#### Infrared Spectra of Suspension Media

As it is difficult to prepare pellets and thin mineral oil films of reproducible thickness, the bands of these suspension matrixes are always found superimposed on the sample spectra.

Mineral oil (nujol): 10  $\mu\text{m}$  thickness



Potassium bromide: pellet



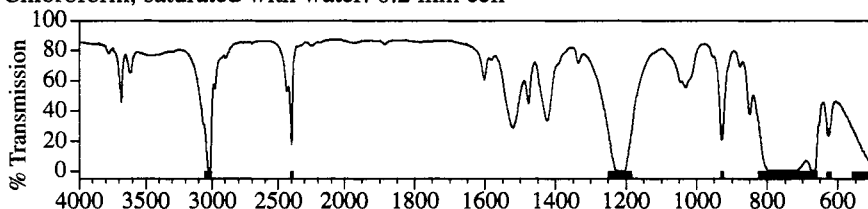
### 6.14.3

#### Interferences in Infrared Spectra

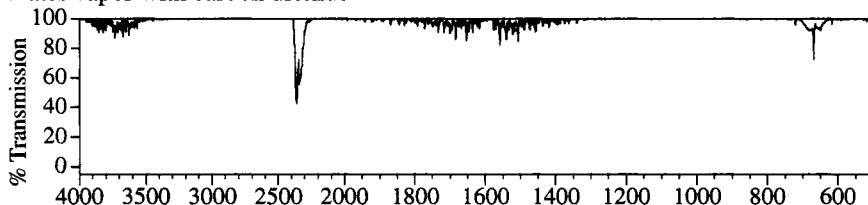
Traces of water in carbon tetrachloride or chloroform may give rise to two bands in the vicinity of  $3700$  and  $3600\text{ cm}^{-1}$  as well as one around  $1600\text{ cm}^{-1}$ . At higher concentrations, a broad band at  $3450\text{ cm}^{-1}$  is found. Water in the vapor phase exhibits many sharp bands between  $2000$  and  $1280\text{ cm}^{-1}$ . If present in high concentrations, they may temporarily block the detector and appear as shoulders if occurring at a steep side of a strong signal.

Dissolved carbon dioxide shows an absorption band at  $2325\text{ cm}^{-1}$ . In solutions that contain amines and traces of water,  $\text{CO}_2$  can form carbonates, which lead to the appearance of unexpected bands of protonated N-containing groups. In improperly balanced double beam instruments, gaseous  $\text{CO}_2$  can give rise to two signals at approximately  $2360$  and  $2335\text{ cm}^{-1}$  as well as a signal at  $667\text{ cm}^{-1}$ .

Chloroform, saturated with water: 0.2 mm cell



Water vapor with carbon dioxide



Commercially available polymers often contain phthalates as plasticizers, which can be found in apparently pure samples and give rise to a band at  $1725\text{ cm}^{-1}$ . The presence of such phthalates can be confirmed by MS ( $m/z$  149). In the course of chemical reactions, phthalates may be transformed into phthalic anhydride, which shows a band at  $1755\text{ cm}^{-1}$ .

Other frequently encountered contaminants are silicones, which generally exhibit a band at  $1625\text{ cm}^{-1}$ , together with a broad signal in the region from  $1100$  to  $1000\text{ cm}^{-1}$ .