

## LAMPIRAN III

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468 Chapter 10 Infrared and Raman Spectrometries: Vibrational Spectrometries

**Table 10B.2** Simplified Correlation Chart of Molecular Vibrations by Type\*

Type of vibration		Frequency (cm <sup>-1</sup> )	Intensity <sup>†</sup>	
C—H	Alkanes (stretch)	3000–2850	s	
	—CH <sub>3</sub> (bend)	1450 and 1375	m	
	—CH <sub>2</sub> — (bend)	1465	m	
	Alkenes	(stretch)	3100–3000	m
		(out-of-plane bend)	1000–650	s
	Aromatics	(stretch)	3150–3050	s
		(out-of-plane bend)	900–690	s
	Alkyne (stretch)	ca. 3300	s	
	Aldehyde		2900–2800	w
			2800–2700	w
C—C	Alkane	not interpretatively useful		
C=C	Alkene	1680–1600	m-w	
	Aromatic	1600 and 1475	m-w	
C≡C	Alkyne	2250–2100	m-w	
C=O	Aldehyde	1740–1720	s	
	Ketone	1725–1705	s	
	Carboxylic acid	1725–1700	s	
	Ester	1750–1730	s	
	Amide	1670–1640	s	
	Anhydride	1810 and 1760	s	
	Acid chloride	1800	s	
C—O	Alcohols, ethers, esters, carboxylic acids, anhydrides	1300–1000	s	
O—H	Alcohols, phenols			
	Free	3650–3600	m	
	H-bonded	3500–3200	m	
	Carboxylic acids	3400–2400	m	
N—H	Primary and secondary amines and amides (stretch)	3500–3100	m	
	(bend)	1640–1550	m-s	
C—N	Amines	1350–1000	m-s	
C=N	Imines and oximes	1690–1640	w-s	
C≡N	Nitriles	2260–2240	m	
X=C=Y	Allenes, ketenes, isocyanates, isothiocyanates	2270–1950	m-s	
N=O	Nitro (R—NO <sub>2</sub> )	1550 and 1350	s	
S—H	Mercaptans	2550	w	
S=O	Sulfoxides	1050	s	
	Sulfones, sulfonyl chlorides	1375–1300 and	s	
	Sulfates, sulfonamides	1200–1140	s	
C—X	Fluoride	1400–1000	s	
	Chloride	800–600	s	
	Bromide, iodide	<667	s	

\*Data from Pavia, D. L., Lampman, G. M., Kriz, G. S. 1979. *Introduction to Spectroscopy: A Guide for Students of Organic Chemistry*.

<sup>†</sup>s = strong, m = medium, w = weak.

**TABLE 7-3 A Numerical Listing of Wavenumber Ranges in Which Some Functional Groups and Classes of Compounds Absorb in the Infrared**

Range (cm <sup>-1</sup> ) and Intensity <sup>a</sup>	Group and Class	Assignment and Remarks
3700-3600 (s)	-OH in alcohols and phenols	OH stretch (dil soln)
3520-3320 (m-s)	-NH <sub>2</sub> in aromatic amines, primary amines and amides	NH stretch (dil soln)
3420-3250 (s)	-OH in alcohols and phenols	OH stretch (solids & liquids)
3360-3340 (m)	-NH <sub>2</sub> in primary amides	NH <sub>2</sub> antisym stretch (solids)
3320-3250 (m)	-OH in oximes	O-H stretch
3300-3250 (m-s)	≡CH in acetylenes	≡CH-H stretch
3300-3280 (s)	-NH in secondary amides	NH stretch (solids); also in polypeptides and proteins
3200-3180 (s)	-NH <sub>2</sub> in primary amides	NH <sub>2</sub> sym stretch (solids)
3200-3000 (v br)	-NH <sub>3</sub> <sup>+</sup> in amino acids	NH <sub>3</sub> <sup>+</sup> antisym stretch
3100-2400 (v br)	-OH in carboxylic acids	H-bonded OH stretch
3100-3000 (m)	=CH in aromatic and unsaturated hydrocarbons	=C-H stretch
2990-2850 (m-s)	-CH <sub>3</sub> and -CH <sub>2</sub> - in aliphatic compounds	CH antisym and sym stretching
2850-2700 (m)	-CH <sub>3</sub> attached to O or N	CH stretching modes
2750-2650 (w-m)	-CHO in aldehydes	overtone of CH bending (Fermi resonance)
2750-2350 (br)	-NH <sub>3</sub> <sup>+</sup> in amine hydrohalides	NH stretching modes
2720-2560 (m)	-OH in phosphorus oxyacids	associated OH stretching
2600-2540 (w)	-SH in alkyl mercaptans	S-H stretch; strong in Raman
2410-2280 (m)	-PH in phosphines	P-H stretch; sharp peak
2300-2230 (m)	N≡N in diazonium salts	N≡N stretch, aq soln
2285-2250 (s)	N=C=O in isocyanates	N=C=O antisym stretch
2260-2200 (m-s)	C≡N in nitriles	C≡N stretch
2260-2190 (w-m)	C≡C in alkynes (disubst)	C≡C stretch; strong in Raman
2190-2130 (m)	C≡N in thiocyanates	C≡N stretch
2175-2115 (s)	N≡C in isonitriles	N≡C stretch
2160-2080 (m)	N=N=N in azides	N=N=N antisym stretch
2140-2100 (w-m)	C≡C in alkynes (monosubst)	C≡C stretch
2000-1650 (w)	substituted benzene rings	several bands from overtone and combination bands
1980-1950 (s)	C=C=C in allenes	C=C=C antisym stretch
1870-1650 (vs)	C=O in carbonyl compounds	C=O stretch
1870-1830 (s)	C=O in β-lactones	C=O stretch
1870-1790 (vs)	C=O in anhydrides	C=O antisym stretch; part of doublet
1820-1800 (s)	C=O in acid halides	C=O stretch; lower for aromatic acid halides
1780-1760 (s)	C=O in γ-lactones	C=O stretch
1765-1725 (vs)	C=O in anhydrides	C=O sym stretch; part of doublet
1760-1740 (vs)	C=O in α-keto esters	C=O stretch; enol form
1750-1730 (s)	C=O in δ-lactones	C=O stretch
1750-1740 (vs)	C=O in esters	C=O stretch; 20 cm <sup>-1</sup> lower if unsaturated
1740-1720 (s)	C=O in aldehydes	C=O stretch; 30 cm <sup>-1</sup> lower if unsaturated
1720-1700 (s)	C=O in ketones	C=O stretch; 20 cm <sup>-1</sup> lower if unsaturated
1710-1690 (s)	C=O in carboxylic acids	C=O stretch; fairly broad
1690-1640 (s)	C=N in oximes	C=N stretch; also imines
1680-1620 (s)	C=O and NH <sub>2</sub> in primary amides	two bands from C=O stretch and NH <sub>2</sub> deformation
1680-1635 (s)	C=O in ureas	C=O stretch; broad band
1680-1630 (m-s)	C=C in alkenes, etc.	C=C stretch
1680-1630 (vs)	C=O in secondary amides	C=O stretch (Amide I band)

<sup>a</sup>v = very, s = strong, m = medium, w = weak, br = broad.

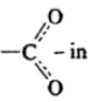
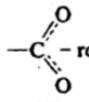
TABLE 7-3 (Continued)

Range (cm <sup>-1</sup> ) and Intensity*	Group and Class	Assignment and Remarks
1670-1640 (s-vs)	C=O in benzophenones	C=O stretch
1670-1650 (vs)	C=O in primary amides	C=O stretch (Amide I band)
1670-1630 (vs)	C=O in tertiary amides	C=O stretch
1655-1635 (vs)	C=O in $\beta$ -ketone esters	C=O stretch; enol form
1650-1620 (w-m)	N-H in primary amides	NH deformation (Amide II band)
1650-1580 (m-s)	NH <sub>2</sub> in primary amines	NH <sub>2</sub> deformation
1640-1580 (s)	NH <sub>3</sub> <sup>+</sup> in amino acids	NH <sub>3</sub> deformation
1640-1580 (vs)	C=O in $\beta$ -diketones	C=O stretch; enol form
1620-1610 (s)	C=C in vinyl ethers	C=C stretch; doublet due to rotational isomerism
1615-1590 (m)	benzene ring in aromatic compounds	ring stretch; sharp peak
1615-1565 (s)	pyridine derivatives	ring stretch; doublet
1610-1580 (s)	NH <sub>2</sub> in amino acids	NH <sub>2</sub> deformation; broad band
1610-1560 (vs)	COO <sup>-</sup> in carboxylic acid salts	$\begin{array}{c} \text{O} \\ \parallel \\ \text{---C---} \\ \parallel \\ \text{O} \end{array}$ antisym stretch
1590-1580 (m)	NH <sub>2</sub> primary alkyl amide	NH <sub>2</sub> deformation (Amide II band)
1575-1545 (vs)	NO <sub>2</sub> in aliphatic nitro compounds	NO <sub>2</sub> antisym stretch
1565-1475 (vs)	NH in secondary amides	NH deformation (Amide II band)
1560-1510 (s)	triazine compounds	ring stretch; sharp band
1550-1490 (s)	NO <sub>2</sub> in aromatic nitro compounds	NO <sub>2</sub> antisym stretch
1530-1490 (s)	NH <sub>3</sub> <sup>+</sup> in amino acids or hydrochlorides	NH <sub>3</sub> <sup>+</sup> deformation
1530-1450 (m-s)	N=N-O in azoxy compounds	N=N-O antisym stretch
1515-1485 (m)	benzene ring in aromatic compounds	ring stretch, sharp band
1475-1450 (vs)	CH <sub>2</sub> in aliphatic compounds	CH <sub>2</sub> scissors vibration
1465-1440 (vs)	CH <sub>3</sub> in aliphatic compounds	CH <sub>3</sub> antisym deformation
1440-1400 (m)	OH in carboxylic acids	in-plane OH bending
1420-1400 (m)	C-N in primary amides	C-N stretch (Amide III band)
1400-1370 (m)	<i>t</i> -butyl group	CH <sub>3</sub> deformations (two bands)
1400-1310 (s)	COO <sup>-</sup> group in carboxylic acid salts	$\begin{array}{c} \text{O} \\ \parallel \\ \text{C---} \\ \parallel \\ \text{O} \end{array}$ sym stretch; broad band
1390-1360 (vs)	SO <sub>2</sub> in sulfonyl chlorides	SO <sub>2</sub> antisym stretch
1380-1370 (s)	CH <sub>3</sub> in aliphatic compounds	CH <sub>3</sub> sym deformation
1380-1360 (m)	isopropyl group	CH <sub>3</sub> deformations (two bands)
1375-1350 (s)	NO <sub>2</sub> in aliphatic nitro compounds	NO <sub>2</sub> sym stretch
1360-1335 (vs)	SO <sub>2</sub> in sulfonamides	SO <sub>2</sub> antisym stretch
1360-1320 (vs)	NO <sub>2</sub> in aromatic nitro compounds	NO <sub>2</sub> sym stretch
1350-1280 (m-s)	N=N-O in azoxy compounds	N=N-O sym stretch
1335-1295 (vs)	SO <sub>2</sub> in sulfones	SO <sub>2</sub> antisym stretch
1330-1310 (m-s)	CF <sub>3</sub> attached to a benzene ring	CF <sub>3</sub> antisym stretch
1300-1200 (vs)	$\overset{+}{\text{N}}-\overset{-}{\text{O}}$ in pyridine <i>N</i> -oxides	N-O stretch
1300-1175 (vs)	P=O in phosphorus oxyacids and phosphates	P=O stretch
1300-1000 (vs)	C-F in aliphatic fluoro compounds	C-F stretch
1285-1240 (vs)	Ar-O in alkyl aryl ethers	C-O stretch
1280-1250 (vs)	Si-CH <sub>3</sub> in silanes	CH <sub>3</sub> sym deformation
1280-1240 (m-s)	C-C in epoxides	C-O stretch
1280-1180 (s)	C-N in aromatic amines	C-N stretch
1280-1150 (vs)	C-O-C in esters, lactones	C-O-C antisym stretch

TABLE 7-3 (Continued)

Range (cm <sup>-1</sup> ) and Intensity <sup>a</sup>	Group and Class	Assignment and Remarks
1255-1240 (m)	<i>t</i> -butyl in hydrocarbons	skeletal vibration; second band near 1200 cm <sup>-1</sup>
1245-1155 (vs)	SO <sub>3</sub> H in sulfonic acids	S=O stretch
1240-1070 (s-vs)	C—O—C in ethers	C—O—C stretch; also in esters
1230-1100 (s)	C—C—N in amines	C—C—N bending
1225-1200 (s)	C—O—C in vinyl ethers	C—O—C antisym stretch
1200-1165 (s)	SO <sub>2</sub> Cl in sulfonyl chlorides	SO <sub>2</sub> sym stretch
1200-1015 (vs)	C—OH in alcohols	C—O stretch
1170-1145 (s)	SO <sub>2</sub> NH <sub>2</sub> in sulfonamides	SO <sub>2</sub> sym stretch
1170-1140 (s)	SO <sub>2</sub> — in sulfones	SO <sub>2</sub> sym stretch
1160-1100 (m)	C=S in thiocarbonyl compounds	C=S stretch; strong in Raman
1150-1070 (vs)	C—O—C in aliphatic ethers	C—O—C antisym stretch
1120-1080 (s)	C—O—H in secondary or tertiary alcohols	C—O stretch
1120-1030 (s)	C—NH <sub>2</sub> in primary aliphatic amines	C—N stretch
1100-1000 (vs)	Si—O—Si in siloxanes	Si—O—Si antisym stretch
1080-1040 (s)	SO <sub>3</sub> H in sulfonic acids	SO <sub>3</sub> sym stretch
1065-1015 (s)	CH—O—H in cyclic alcohols	C—O stretch
1060-1025 (vs)	CH <sub>2</sub> —O—H in primary alcohols	C—O stretch
1060-1045 (vs)	S=O in alkyl sulfoxides	S=O stretch
1055-915 (vs)	P—O—C in organophosphorus compounds	P—O—C antisym stretch
1030-950 (w)	carbon ring in cyclic compounds	ring breathing mode; strong in Raman
1000-950 (s)	CH=CH <sub>2</sub> in vinyl compounds	=CH out-of-plane deformation
980-960 (vs)	CH=CH— in trans disubstituted alkenes	=CH out-of-plane deformation
950-900 (vs)	CH=CH <sub>2</sub> in vinyl compounds	CH <sub>2</sub> out-of-plane wag
900-865 (vs)	$\begin{array}{c} \text{R} \\   \\ \text{CH}_2=\text{C} \\   \\ \text{R}' \end{array}$ in vinylidenes	CH <sub>2</sub> out-of-plane wag
890-805 (vs)	1,2,4-trisubst benzenes	CH out-of-plane deformation (two bands)
860-760 (vs, br)	R—NH <sub>2</sub> primary amines	NH <sub>2</sub> wag
860-720 (vs)	Si—C in organosilicon compounds	Si—C stretch
850-830 (vs)	1,3,5-trisubst benzenes	CH out-of-plane deformation
850-810 (vs)	Si—CH <sub>3</sub> in silanes	Si—CH <sub>3</sub> rocking
850-790 (m)	$\begin{array}{c} \text{R} \\   \\ \text{CH}=\text{C} \\   \\ \text{R}' \end{array}$ in trisubst alkenes	CH out-of-plane deformation
850-550 (m)	C—Cl in chloro compounds	C—Cl stretch
830-810 (vs)	<i>p</i> -disubst benzenes	CH out-of-plane deformation
825-805 (vs)	1,2,4-trisubst benzenes	CH out-of-plane deformation
820-800 (s)	triazines	CH out-of-plane deformation
815-810 (s)	CH=CH <sub>2</sub> in vinyl ethers	CH <sub>2</sub> out-of-plane wag
810-790 (vs)	1,2,3,4-tetrasubst benzenes	CH out-of-plane deformation
800-690 (vs)	<i>m</i> -disubst benzenes	CH out-of-plane deformation (two bands)
785-680 (vs)	1,2,3-trisubst benzenes	CH out-of-plane deformation (two bands)
775-650 (m)	C—S in sulfonyl chlorides	C—S stretch; strong in Raman
770-690 (vs)	monosubst benzenes	CH out-of-plane deformation (two bands)
760-740 (s)	<i>o</i> -disubst benzenes	CH out-of-plane deformation
760-510 (s)	C—Cl alkyl chlorides	C—Cl stretch
740-720 (w-m)	—(CH <sub>2</sub> ) <sub><i>n</i></sub> — in hydrocarbons	CH <sub>2</sub> rocking in methylene chains; intensity depends on chain length
730-665 (s)	CH=CH in cis disubst alkenes	CH out-of-plane deformation
720-600 (s, br)	Ar—OH in phenols	OH out-of-plane deformation

TABLE 7-3 (Continued)

Range (cm <sup>-1</sup> ) and Intensity <sup>a</sup>	Group and Class	Assignment and Remarks
710-570 (m)	C-S in sulfides	C-S stretch; strong in Raman
700-590 (s)	O-C=O in carboxylic acids	O-C=O bending
695-635 (s)	C-C-CHO in aldehydes	C-C-CHO bending
680-620 (s)	C-OH in alcohols	C-O-H bending
680-580 (s)	C≡C-H in alkynes	C≡C-H bending
650-600 (w)	S-C≡N in thiocyanates	S-C stretch; strong in Raman
650-600 (s)	NO <sub>2</sub> in aliphatic nitro compounds	NO <sub>2</sub> deformation
650-500 (s)	Ar-CF <sub>3</sub> in aromatic trifluoro-methyl compounds	CF <sub>3</sub> deformation (two or three bands)
650-500 (s)	C-Br in bromo compounds	C-Br stretch
645-615 (m-s)	naphthalenes	in-plane ring deformation
645-575 (s)	O-C-O in esters	O-C-O bend
640-630 (s)	=CH <sub>2</sub> in vinyl compounds	=CH <sub>2</sub> twisting
635-605 (m-s)	pyridines	in-plane ring deformation
630-570 (s)	N-C=O in amides	N-C=O bend
630-565 (s)	C-CO-C in ketones	C-CO-C bend
615-535 (s)	C=O in amides	C=O out-of-plane bend
610-565 (vs)	SO <sub>2</sub> in sulfonyl chlorides	SO <sub>2</sub> deformation
610-545 (m-s)	SO <sub>2</sub> in sulfones	SO <sub>2</sub> scissoring
600-465 (s)	C-I in iodo compounds	C-I stretch
580-530 (m-s)	C-C-CN in nitriles	C-C-CN bend
580-520 (m)	NO <sub>2</sub> in aromatic nitro compounds	NO <sub>2</sub> deformation
580-430 (s)	ring in cycloalkanes	ring deformation
580-420 (m-s)	ring in benzene derivatives	in-plane and out-of-plane ring deformations (two bands)
570-530 (vs)	SO <sub>2</sub> in sulfonyl chlorides	SO <sub>2</sub> rocking
565-520 (s)	C-C=O in aldehydes	C-C=O bend
565-440 (w-m)	C <sub>n</sub> H <sub>2n+1</sub> in alkyl groups	chain deformation modes (two bands)
560-510 (s)	C-C=O in ketones	C-C=O bend
560-500 (s)	 - in amino acids	 rocking
555-545 (s)	=CH <sub>2</sub> in vinyl compounds	=CH <sub>2</sub> twisting
550-465 (s)	C-C=O in carboxylic acids	C-C=O bend
545-520 (s)	naphthalenes	in-plane ring deformation
530-470 (m-s)	NO <sub>2</sub> in nitro compounds	NO <sub>2</sub> rocking
520-430 (m-s)	C-O-C in ethers	C-O-C bend
510-400 (s)	C-N-C in amines	C-N-C bend
490-465 (variable)	naphthalenes	out-of-plane ring bending
440-420 (s)	Cl-C=O in acid chlorides	Cl-C=O in-plane deformation
405-400 (s)	S-C≡N in thiocyanates	S-C≡N bend

Joseph B. Lambert, et al.  
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