

LAMPIRAN II

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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^{-1})	Intensity [†]
C—H	Alkanes	(stretch)	3000–2850	s
	$\begin{array}{c} \text{CH}_3 \\ \\ -\text{CH}- \end{array}$	(bend)	1450 and 1375	m
	$-\text{CH}_2-$	(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=C	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—C	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=C	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 ₂)		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*.

[†]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^{-1}) and Intensity*	Group and Class	Assignment and Remarks
3700–3600 (s)	—OH in alcohols and phenols	OH stretch (dil soln)
3520–3320 (m-s)	—NH ₂ 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 ₂ in primary amides	NH ₂ 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 ₂ in primary amides	NH ₂ sym stretch (solids)
3200–3000 (v br)	—NH ₃ ⁺ in amino acids	NH ₃ ⁺ 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 ₃ and —CH ₂ — in aliphatic compounds	CH antisym and sym stretching
2850–2700 (m)	—CH ₃ 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 ₃ ⁺ 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= 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^{-1} lower if unsaturated
1740–1720 (s)	C=O in aldehydes	C=O stretch; 30 cm^{-1} lower if unsaturated
1720–1700 (s)	C=O in ketones	C=O stretch; 20 cm^{-1} 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 ₂ in primary amides	two bands from C=O stretch and NH ₂ 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)

*v = very, s = strong, m = medium, w = weak, br = broad.

TABLE 7-3 (Continued)

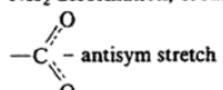
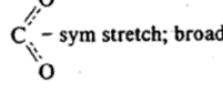
Range (cm^{-1}) and Intensity ^a	Group and Class	Assignment and Remarks
1670–1640 (s-vs)	C=O in benzophenones	C=O stretch
1670–1650 (vs)	C=O in primary amides	C=O stretch (Amide I band)
1670–1630 (vs)	C=O in tertiary amides	C=O stretch
1655–1635 (vs)	C=O in β -ketone esters	C=O stretch; enol form
1650–1620 (w-m)	N—H in primary amides	NH deformation (Amide II band)
1650–1580 (m-s)	NH ₂ in primary amines	NH ₂ deformation
1640–1580 (s)	NH ₃ ⁺ in amino acids	NH ₃ deformation
1640–1580 (vs)	C=O in β -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 ₂ in amino acids	NH ₂ deformation; broad band
1610–1560 (vs)	COO ⁻ in carboxylic acid salts	
1590–1580 (m)	NH ₂ primary alkyl amide	NH ₂ deformation (Amide II band)
1575–1545 (vs)	NO ₂ in aliphatic nitro compounds	NO ₂ 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 ₂ in aromatic nitro compounds	NO ₂ antisym stretch
1530–1490 (s)	NH ₃ ⁺ in amino acids or hydrochlorides	NH ₃ ⁺ 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 ₂ in aliphatic compounds	CH ₂ scissors vibration
1465–1440 (vs)	CH ₃ in aliphatic compounds	CH ₃ 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)	t-butyl group	CH ₃ deformations (two bands)
1400–1310 (s)	COO ⁻ group in carboxylic acid salts	
1390–1360 (vs)	SO ₂ in sulfonyl chlorides	SO ₂ antisym stretch
1380–1370 (s)	CH ₃ in aliphatic compounds	CH ₃ sym deformation
1380–1360 (m)	isopropyl group	CH ₃ deformations (two bands)
1375–1350 (s)	NO ₂ in aliphatic nitro compounds	NO ₂ sym stretch
1360–1335 (vs)	SO ₂ in sulfonamides	SO ₂ antisym stretch
1360–1320 (vs)	NO ₂ in aromatic nitro compounds	NO ₂ sym stretch
1350–1280 (m-s)	N=N—O in azoxy compounds	N=N—O sym stretch
1335–1295 (vs)	SO ₂ in sulfones	SO ₂ antisym stretch
1330–1310 (m-s)	CF ₃ attached to a benzene ring	CF ₃ antisym stretch
1300–1200 (vs)	N— \bar{O} in pyridine N-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 ₃ in silanes	CH ₃ 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)

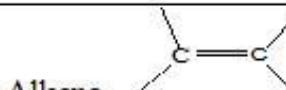
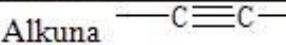
Range (cm^{-1}) and Intensity*	Group and Class	Assignment and Remarks
1255-1240 (m)	t-butyl in hydrocarbons	skeletal vibration; second band near 1200 cm^{-1}
1245-1155 (vs)	SO_3H in sulfonic acids	$\text{S}=\text{O}$ stretch
1240-1070 (s-vs)	$\text{C}-\text{O}-\text{C}$ in ethers	$\text{C}-\text{O}-\text{C}$ stretch; also in esters
1230-1100 (s)	$\text{C}-\text{C}-\text{N}$ in amines	$\text{C}-\text{C}-\text{N}$ bending
1225-1200 (s)	$\text{C}-\text{O}-\text{C}$ in vinyl ethers	$\text{C}-\text{O}-\text{C}$ antisym stretch
1200-1165 (s)	SO_2Cl in sulfonyl chlorides	SO_2 sym stretch
1200-1015 (vs)	$\text{C}-\text{OH}$ in alcohols	$\text{C}-\text{O}$ stretch
1170-1145 (s)	SO_2NH_2 in sulfonamides	SO_2 sym stretch
1170-1140 (s)	SO_2- in sulfones	SO_2 sym stretch
1160-1100 (m)	$\text{C}=\text{S}$ in thiocarbonyl compounds	$\text{C}=\text{S}$ stretch; strong in Raman
1150-1070 (vs)	$\text{C}-\text{O}-\text{C}$ in aliphatic ethers	$\text{C}-\text{O}-\text{C}$ antisym stretch
1120-1080 (s)	$\text{C}-\text{O}-\text{H}$ in secondary or tertiary alcohols	$\text{C}-\text{O}$ stretch
1120-1030 (s)	$\text{C}-\text{NH}_2$ in primary aliphatic amines	$\text{C}-\text{N}$ stretch
1100-1000 (vs)	$\text{Si}-\text{O}-\text{Si}$ in siloxanes	$\text{Si}-\text{O}-\text{Si}$ antisym stretch
1080-1040 (s)	SO_3H in sulfonic acids	SO_3 sym stretch
1065-1015 (s)	$\text{CH}-\text{O}-\text{H}$ in cyclic alcohols	$\text{C}-\text{O}$ stretch
1060-1025 (vs)	$\text{CH}_2-\text{O}-\text{H}$ in primary alcohols	$\text{C}-\text{O}$ stretch
1060-1045 (vs)	$\text{S}=\text{O}$ in alkyl sulfoxides	$\text{S}=\text{O}$ stretch
1055-915 (vs)	$\text{P}-\text{O}-\text{C}$ in organophosphorus compounds	$\text{P}-\text{O}-\text{C}$ antisym stretch
1030-950 (w)	carbon ring in cyclic compounds	ring breathing mode; strong in Raman
1000-950 (s)	$\text{CH}=\text{CH}_2$ in vinyl compounds	$=\text{CH}$ out-of-plane deformation
980-960 (vs)	$\text{CH}=\text{CH}-$ in trans disubstituted alkenes	$=\text{CH}$ out-of-plane deformation
950-900 (vs)	$\text{CH}=\text{CH}_2$ in vinyl compounds	CH_2 out-of-plane wag
900-865 (vs)	$\begin{array}{c} \text{R} \\ \\ \text{CH}_2=\text{C} \\ \\ \text{R}' \end{array}$ in vinylidenes	CH_2 out-of-plane wag
890-805 (vs)	1,2,4-trisubst benzenes	CH out-of-plane deformation (two bands)
860-760 (vs, br)	$\text{R}-\text{NH}_2$ primary amines	NH_2 wag
860-720 (vs)	$\text{Si}-\text{C}$ in organosilicon compounds	$\text{Si}-\text{C}$ stretch
850-830 (vs)	1,3,5-trisubst benzenes	CH out-of-plane deformation
850-810 (vs)	$\text{Si}-\text{CH}_3$ in silanes	$\text{Si}-\text{CH}_3$ 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)	$\text{C}-\text{Cl}$ in chloro compounds	$\text{C}-\text{Cl}$ stretch
830-810 (vs)	p-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)	$\text{CH}=\text{CH}_2$ in vinyl ethers	CH_2 out-of-plane wag
810-790 (vs)	1,2,3,4-tetrasubst benzenes	CH out-of-plane deformation
800-690 (vs)	m-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)	$\text{C}-\text{S}$ in sulfonyl chlorides	$\text{C}-\text{S}$ 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)	$\text{C}-\text{Cl}$ alkyl chlorides	$\text{C}-\text{Cl}$ stretch
740-720 (w-m)	$-(\text{CH}_2)_n-$ in hydrocarbons	CH_2 rocking in methylene chains; intensity depends on chain length
730-665 (s)	$\text{CH}=\text{CH}$ in cis disubst alkenes	CH out-of-plane deformation
720-600 (s, br)	$\text{Ar}-\text{OH}$ in phenols	OH out-of-plane deformation

TABLE 7-3 (Continued)

Range (cm^{-1}) and Intensity*	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 ₂ in aliphatic nitro compounds	NO ₂ deformation
650–500 (s)	Ar—CF ₃ in aromatic trifluoro-methyl compounds	CF ₃ 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 ₂ in vinyl compounds	=CH ₂ 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 ₂ in sulfonyl chlorides	SO ₂ deformation
610–545 (m-s)	SO ₂ in sulfones	SO ₂ 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 ₂ in aromatic nitro compounds	NO ₂ 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 ₂ in sulfonyl chlorides	SO ₂ rocking
565–520 (s)	C—C=O in aldehydes	C—C=O bend
565–440 (w-m)	C _n H _{2n+1} 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 ₂ in vinyl compounds	=CH ₂ 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 ₂ in nitro compounds	NO ₂ 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.

Introduction to Organic
Spectroscopy, Macmillan
 Publ. N.Y. (1987)

Ikatan	Tipe Senyawa	Daerah frekuensi (cm ⁻¹)	Intensitas
C - H	Alkana	2850 – 2970 1340 - 1470	Kuat Kuat
C - H	Alkena 	3010 – 3095 675 - 995	Sedang Kuat
C - H	Alkuna 	3300	Kuat
C - H	Cincin Aromatik	3010 – 3100 690 – 900	Sedang Kuat
O - H	Fenol, monomer alkohol, alkohol ikatan hidrogen, fenol monomer asam karboksilat, ikatan hidrogen asam karboksilat	3590 – 3650 3200 – 3600 3500 – 3650 2500 - 2700	Berubah-ubah Berubah-ubah, terkadang melebar Sedang Melebar
N - H	Amina, Amida	3300 – 3500	Sedang
C ≡ C	Alkena	1610 – 1680	Berubah-ubah
C ≡ C	Cincin Aromatik	1500 – 1600	Berubah-ubah
C ≡ C	Alkuna	2100 – 2260	Berubah-ubah
C - N	Amina, Amida	1180 – 1360	Kuat
C ≡ N	Nitril	2210 – 2280	Kuat
C - O	Alkohol, Eter, Asam Karborsilat, Ester	1050 – 1300	Kuat
C ≡ O	Aldehid, Keton, Asam Karboksilat, Ester	1690 – 1760	Kuat
NO ₂	Senyawa Nitro	1500 – 1570 1300 - 1370	Kuat Kuat

Sumber : *Principle of Instrumental Analysis*, Skoog, Holler, Nieman, 1998.