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Organic Chemistry

Appendix B

Reference tables for interpreting infrared spectra

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Appendix B

Infrared Spectral Tables

Group	Intensity ^a	Range (cm ⁻¹) ^b	Group	Intensity ^a	Range (cm ⁻¹) ^b
Hydrocarbons			Alkene, nonconjugated		
C—H Stretching			Monosubstituted		
Alkane	m-s	2960-2850	Disubstituted, <i>cis</i>	m	~1645
Alkene, monosubstituted	m	3040-3010	Disubstituted, <i>trans</i>	m	~1658
	and m	3095-3075	Disubstituted, <i>gem</i>	m	~1675
Alkene, disubstituted, <i>cis</i>	m	3040-3010	Trisubstituted	m	~1653
Alkene, disubstituted, <i>trans</i>	m	3040-3010	Tetrasubstituted	w	~1669
Alkene, disubstituted, <i>gem</i>	m	3095-3075	Diene	w	~1669
Alkene, trisubstituted	m	3040-3010		and w	~1650
Alkyne	s	~3300	Alkyne, monosubstituted	m	~1600
Aromatic	v	~3030	Alkyne, disubstituted	v,w	2140-2100
C—H Bending			Allene	m	2260-2190
Alkane, C—H	w	~1340		and m	~1960
Alkane, —CH ₂ —	m	1485-1445	Aromatic	v	~1060
Alkane, —CH ₃	m	1470-1430		v	~1600
	and s	1380-1370		m	~1580
Alkane, <i>gem</i> -dimethyl	s	1385-1380		and m	~1500
	and s	1370-1365	Carbonyl Groups		
Alkane, <i>tert</i> -butyl	m	1395-1385	Ketone		
	and s	1370-1365	Acyclic	s	1725-1705
Alkene, monosubstituted	s	1420-1410	Cyclic, 6-member ring or larger	s	1725-1705
	s	995-985	Cyclic, 5-member ring	s	1750-1740
	and s	915-905	Cyclic, 4-member ring	s	~1775
Alkene, disubstituted, <i>cis</i>	s	~690	α,β -Unsaturated, acyclic	s	1685-1665
Alkene, disubstituted, <i>trans</i>	m	1310-1295	α,β -Unsaturated, cyclic, 6-member ring or larger	s	1685-1665
	and s	970-960	α,β -Unsaturated, acyclic, 5-member ring	s	1725-1708
Alkene, disubstituted, <i>gem</i>	s	1420-1410	$\alpha,\beta,\alpha',\beta'$ -Unsaturated, acyclic	s	1670-1663
	and s	895-885	Aryl	s	1700-1680
Alkene, trisubstituted	s	840-790	Diaryl	s	1670-1660
Alkyne	s	~630	α -Diketones	s	1730-1710
Aromatic, five adjacent H	v,s	~750	β -Diketones (enolic)	s	1640-1540
	and v,s	~700	1,4-Quinones	s	1690-1660
Aromatic, four adjacent H	v,s	~750	Ketenes	s	~2150
Aromatic, three adjacent H	v,m	~780	Aldehydes		
Aromatic, two adjacent H	v, m	~830	Acyclic	s	1740-1720
Aromatic, one H	v,w	~880	α,β -Unsaturated and aryl	s	1780-1750
α,β -Unsaturated, acyclic	s	1705-1680		and m	1750-1720
$\alpha,\beta,\gamma,\delta$ -Unsaturated, acyclic	s	1680-1660	Ester		
Aryl	s	1715-1695			
Aldehyde C-H	w	2900-2820			
	and w	2775-2700			
C—C Stretching					

Group	Intensity ^a	Range (cm ⁻¹) ^b	Group	Intensity ^a	Range (cm ⁻¹) ^b
Acyclic	s	1750-1735	Ureas, cyclic, 5-membered ring	s	~1720
Cyclic, δ-lactones	s	1750-1735	Urethanes	s	1740-1690
Cyclic, γ-lactones	s	1780-1760	Imides, acyclic	s and s	~1710 ~1700
Cyclic, β-lactones	s	~1820	Imides, cyclic, 6-membered ring	s and s	~1710 ~1700
Vinyl esters	s	1800-1770	Imides, cyclic, α,β-unsaturated 6-membered ring	s and s	~1730 ~1670
α,β-Unsaturated and aryl	s	1730-1717	Imides, cyclic, 5-membered ring	s and s	~1770 ~1700
α,β-Unsaturated δ-lactone	s	1730-1717	Imides, cyclic, α,β-unsaturated 5-membered ring	s and s	~1790 ~1710
α,β-Unsaturated γ-lactone	s	1760-1740	Amide N—H stretch		
β,γ-Unsaturated γ-lactone	s	~1800	Primary, free	m and m	~3500 ~3400
α-Ketoester	s	1755-1740	Primary, H-bonded	m and m	~3350 ~3180
β-Ketoester (enolic)	s	~1650	Secondary, free	m	~3430
Carbonates	s	1780-1740	Secondary, H-bonded	m	3320-3140
Carboxylic acids			Amide N—H bending		
Acyclic	s	1725-1700	Primary, dilute solution	s	1620-1590
α,β-Unsaturated	s	1715-1690	Secondary	s	1550-1510
Aryl	s	1700-1680	Alcohol O—H stretch		
Hydroxyl stretching (several bands)	w	2700-2500	Free O—H	v, sh	3650-3590
Carboxylate anion	s and s	1610-1550 1400-1300	H-bonded	s,b	3400-3200
Anhydride			Alcohol O—H bending		
Acyclic	s and s	1850-1800 1790-1740	Primary alcohols	s and s	1350-1260 ~1050
α,β-Unsaturated and aryl, acyclic	s and s	1830-1780 1770-1720	Secondary alcohols	s and s	1350-1260 ~1100
Saturated 5-membered ring	s and s	1870-1820 1800-1750	Tertiary alcohols	s and s	1410-1310 ~1150
α,β-Unsaturated 5-membered ring	s and s	1850-1800 1830-1780	Phenols	s and s	1410-1310 ~1200
Acyl halides			Amine N—H stretch		
Acyl fluorides	s	~1850	Primary	m and m	~3500 ~3400
Acyl chlorides	s	~1795	Secondary	m	3500-3310
Acyl bromides	s	~1810	Imine (C=NH)	m	3400-3300
Amide Carbonyls			Amine salts	m	3130-3030
Primary, solid or concentrated solution	s	~1650	Amine N—H bending		
Primary, dilute solution	s	~1690	Primary	s-m	1650-1590
Secondary, solid or concentrated solution	s	1680-1630	Secondary	w	1650-1550
Secondary, dilute solution	s	1700-1670	Amine salts	s and s	1600-1575 ~1500
Tertiary	s	1670-1630			
Cyclic, δ-lactam	s	~1680			
Cyclic, γ-lactam	s	~1700			
Cyclic, γ-lactam, fused to another ring	s	1750-1700			
Cyclic, β-lactam	s	1760-1730			
Cyclic, β-lactam, fused to another ring	s	1780-1770			
Ureas, acyclic	s	~1660			
Ureas, cyclic, 6-membered ring	s	~1640			

Group	Intensity ^a	Range (cm ⁻¹) ^b	Group	Intensity ^a	Range (cm ⁻¹) ^b
Amine C—H vibrations					
Aromatic, primary	s	1340-1250	Nitrates (–ONO ₂)	and s s	1380-1370 1650-1600
Aromatic, secondary	s	1350-1280	Nitrites (–O–N=O)	and s s	1300-1250 1680-1650
Aromatic, tertiary	s	1360-1310		and s	1625-1610
Aliphatic	w and w	~1410 1220-1020	Halogen compounds stretching		
Unsaturated Nitrogen Compounds			Fluorides	s	1400-1000
Alkyl nitriles	m	2260-2240	Chlorides	s	800-600
α,β-Unsaturated alkyl nitriles	m	2235-2215	Bromides	s	600-500
Aryl nitriles	m	2240-2220	Iodides	s	~500
Isocyanates	m	2275-2240	Sulfur compounds		
Isocyanides	m	2220-2070	Thiol S–H stretching	s	2600-2550
Alkyl oximes and imines	v	1690-1640	–C=S stretching	s	1200-1050
α,β-Unsaturated oximes and imines	v	1660-1630	Sulfoxides	s	1070-1030
Azo stretching	v	1630-1575	Sulfones	s and s	1350-1300 1230-1150
Diimide (–N=C=N–)			Sulfites	s s	1430-1350 1230-1150
Stretching	s	2155-2130	Sulfonyl chlorides	s and s	1370-1340 1185-1165
Azide stretching	s and w	2160-2120 1340-1180	Sulfonamides	s and s	1350-1300 1180-1140
Nitroso (C–N=O)	s	1600-1500	Sulfonic acids	s s and s	1210-1150 1060-1030 ~650
Aromatic nitro compounds	s and s	1570-1500 1370-1300			
Aliphatic nitro compounds	s	1570-1550			

^a Abbreviations: s = strong, m = medium, w = weak, v = variable, b = broad, sh = sharp.

^b Abbreviation: ~ = approximately

