

 C_7H_8O



 C_3H_8S











				Inte	ensities ¹
Group		Assignment	Frequency (cm ⁻¹)	IR	R
CH ₃	R-CH ₃	o.ph. str. ²	2975-2950	vs	vs
	"	i.ph. str.	2885-2860	vs	vs
	"	o.ph. bend	1470-1440	ms	ms
	"	i.ph. bend	1380-1370	m	vw
	R-CH(CH ₃) ₂	bend-bend	1385-1380	m	vw
	"	bend-open	1373-1365	m	vw
	R(CH ₃) ₃	bend-bend	1395-1385	m	vw
	"	bend-open	1373-1365	ms	vw
	aryl-CH ₃	i.ph. str. +	2935-2915	ms	ms
	"	bend overtone	2875-2855	m	m
	R-O-CH ₃	i.ph. str.	2850-2815	m	m
	"	i.ph. bend	1450-1430	ms	m
	R ₂ N-CH ₃	i.ph. str	2825-2765	S	s
	O=C-CH ₃	i.ph. bend	1380-1365	S	w
CH ₂	R-CH2-R	o. ph. str. ³	2936-2915	vs	vs
	"	i. ph. str.	2865-2833	vs	vs
	"	Fermi resonance	2920-2890	W	m
	"	bend	1475-1445	ms	ms
	(CH ₂) _{>3}	i.ph. twist	1305-1295	_	m
	(CH ₂) _{>3}	i.ph. rock	726-720	m	_
	$O=C-CH_2$	bend	1445-1405	m	m
	$N \equiv C - CH_2$	bend	1445-1405	m	m
	O-CH ₂	wag	1390-1340	m	m
	Cl-CH ₂	wag	1300-1220	m	m
СН	R ₃ CH	CH bend	1360-1320	W	w
	О=С-Н	CH str. +	2900-2800	m	m
	"	rk overtone	2770-2695	m	m
	"	CH rock	1410-1380	m	m

 $^{1}s = strong, m = medium, w = weak, v = very, br = broad, var. = variable, - = zero$ $^{2}o.ph. str. = out-of-phase stretch, i.ph. str. = in-phase stretch, rk = rock$ $^{3}Note: In the trans zig-zag segments of the long chain (CH₂)_{>6} group, the Raman active CH₂ out-of-phase stretch band is at 2900–2880 cm⁻¹$ (2883 cm⁻¹ in polyethylene). The gauche segments have this at 2936–2916 cm⁻¹ in the Raman.

X-Element	C-C-C-X (i.ph.str.)	$(C)_2C-X$ (i.ph. str.)	(C) ₃ C–X (i. ph. str.)
Carbon (12)	827 cm^{-1}	800 cm^{-1}	733 cm^{-1}
	CH ₃ CH ₂ CH ₂ CH ₃	H ₃ C — CH ₃ CH ₃	$H_3C \longrightarrow CH_3 \\ H_3C \longrightarrow CH_3 \\ CH_3$
Nitrogen (14)	868 cm ⁻¹	802 cm ⁻¹ .CH ₃	748 cm $^{-1}$ CH $_3$
	✓ NH₂	H ₂ N—CH CH ₃	H ₃ C
Oxygen (16)	822 cm^{-1}	819 cm^{-1}	$750~\mathrm{cm}^{-1}$
	ОН	носн сн ₃	СН ₃ Н ₃ С — — ОН СН ₃
Sulfur (32)	670 cm^{-1}	631 cm^{-1}	
	SH	HS-CH ₃ CH ₃	

TABLE 6.2Summary of the Raman In-Phase C-C/C-X Stretching Band for Selected Compounds, where
X is Carbon, Nitrogen, Oxygen or Sulfur

6- 				Inter	sities ¹
Group		Assignment	Frequency (cm ⁻¹)	IR	R
Triple	C–C≡C–H	CH str.	3340-3267	S	w
Bonds	"	$C \equiv C \text{ str.}$	2140-2100	w	vs
	"	CH wag	710-578	s,br	w
	C−C≡C−C	$C \equiv C \text{ str.}$	2245-2100	-	S
	$CH_2 - C \equiv N$	$C \equiv N$ str.	2260-2240	m	vs
	"	CH ₂ bend	1440-1405	m	m
	$conj-C \equiv N$	$C \equiv N \text{ str.}$	2235-2185	var.	S
	S–C≡N	$C \equiv N \text{ str.}$	2170-2135	ms	S

 TABLE 6.3
 Selected Group Frequencies: Triple Bonds, Cumulated Double Bonds, Conjugated Aliphatics and Aromatics

				Inten	sities ¹
Group		Assignment	Frequency (cm ⁻¹)	IR	R
Cumulated	>C=C=CH ₂	CCC o.ph. str.	2000-1900	vs	vw
Double	-N=C=O	NCO o.ph. str.	2300-2250	vs	vw
Bonds	-N=C=S	NCS o.ph. str.	2200-2000	vs	mw
C=C	C=C mono, cis, 1,1	C=C str. ²	1660-1630	m	s
Alkane Subst.	C=C trans, tri, tetra	C=C str. ²	1680-1665	w-o	s
	C=CH-R mono, cis, trans	CH str.	3020-2995	m	m
	C=CH ₂ mono, 1,1	CH ₂ o.ph. str.	3090-3075	m	m
	"	CH ₂ i.ph. str.	3000-2980	m	s
	"	CH ₂ bend	1420-1400	W	m
	R-CH=CH ₂	trans CH i.ph. wag	995-985	s	w
	"	$=CH_2 wag^3$	910-905	s	w
	$R_2C=CH_2$	$=CH_2 wag^3$	900-885	s	w
	R–CH=CH–R trans	=CH i.ph. wag	980-965	s	_
	R–CH=CH–R cis	=CH i.ph. wag	730–650	ms	_
	R-CH=CR ₂	=CH wag	840-790	m	
Aromatics	aryl CH	CH str.	3100-3000	mw	s
	ring	quadrant str.	1620-1585	var	m
	"	quadrant str.	1590-1565	var	m
	"	semicircle str.	1525-1470	var	vw
	"	semicircle str.	1465-1400	m	vw
	mono, meta, 1,3,5	2,4,6 radial i.ph str.	1010-990	vw	vs
	meta, 1,2,4 & 1,3,5	lone H wag	935-810	m	_
	para and 1,2,4	2 adj. H wag	880-795	S	_
	meta and 1,2,3	3 adj. H wag	825-750	S	_
	ortho and mono	4 & 5 adj. H wag	800-725	S	_
	mono, meta, 1,3,5	ring out-of-plane bend	710-665	s	_
	para	ring in-plane bend	650-630	_	m
	mono	ring in-plane bend	630-605	w	m

TABLE 6.3 Selected Group Frequencies: Triple Bonds, Cumulated Double Bonds, Conjugated Aliphatics and Aromatics-cont'd

 $^{1}s = strong, m = medium, w = weak, v = very, br = broad, var. = variable, - = zero$ $^{2}Conjugation lowers C=C frequencies 10-50 cm^{-1} (e.g., N=C-CH=CH_2 1607 cm^{-1})$ $^{3}Electron donor substituents lower the =CH_2 wag frequencies (e.g., R-O-CH=CH_2 813 cm^{-1}) and electron withdrawers raise them (e.g., N=C-CH=CH_2 960 cm^{-1})$

			Intensities ¹	
Pyridine	Assignment	Region (cm ⁻¹)	IR	R
Pyridine	Aryl CH str.	3100-3000	m	m
	Quadrant str.	1615-1570	S	m
	Semi-circle str	1490-1440	S	mw
	2,4,6 carbon radial str.	1035-1025	m	vs
	Ring breath/str.	995-985	m	s
	Quadrant in-plane bend	660-600	_	m
2-Mono- substituted	Quadrant str.	1620-1570	S	m
	Quadrant str.	1580-1560	S	m
	Semi-circle str.	1480-1450	S	m
	Semi-circle str.	1440-1415	S	w
	CH in-plane rk	1050-1040	m	S
	2,4,6 carbon radial str.	1000-985	m	VS
	Quadrant in-plane bend	850-800	W	ms
3-Mono- substituted	Quadrant str.	1595-1570	m	ms
	Quadrant str.	1585-1560	s	m
	Semi-circle str.	1480-1465	S	m
	Semi-circle str.	1430-1410	s	w
	2,4,6 carbon radial str.	1030-1010	m	VS
	Quadrant in-plane bend	805-750	W	m
4-Mono- substituted	Quadrant str.	1605-1565	m	ms
	Quadrant str.	1570-1555	m	m
	Semi-circle str.	1500-1480	m	m
	Semi-circle str.	1420-1410	s	w
	2,4,6 carbon radial str.	1000-985	m	VS
	Quadrant in-plane bend	805-785	W	ms

TABLE 6.7	Selected In-	plane Stretching	g and Bending	Vibrations for P	yridine and Mono	-Subsituted P	yridine
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s = strong, m = medium, w = weak, v = very, var. = variable, - = zero

12- 12-			Intensities ¹	
Pyridine	Assignment	Region (cm ⁻¹)	IR	R
Pyridine	5 adjacent H wag	760-74	S	
	out-of-plane sextant def.	710-700	S	—
2-Mono- substituted	4 adjacent H wag	780-740	S	
3-Mono- substituted	3 adjacent H wag	820-770	S	-
	out-of-plane sextant def	730-690	m-s	W
4-Mono- substituted	2 adjacent H wag	850-790	S	<u>8</u> _0

TABLE 6.8Selected Out-of-plane CH wag and Out-of-plane Sextant Deformation Vibrations for Pyridineand Mono-Subsituted Pyridine

 $^{1}s = strong, m = medium, w = weak, v = very, var. = variable, - = zero$

			Intensities ¹	
Pyridine	Assignment	Region (cm ⁻¹)	IR	R
Pyrrole	NH str.	3500-3000	S	m–w
	=CH str.	3135, 3103	m	S
	Quadrant str. + CH rk	1530	S	
	Quadrant str. + CH rk	1468	m	S
	Semi-circle str $+$ CH rk	1418	m	
	Semi-circle str. + CH rk	1380	S	m
	Ring in-phase str.	1143	m	VS
1-subst pyrrole	Quadrant str.	1560-1540	w-m	m
	Quadrant str.	1510-1490	m	vs
	Semi-circle str.	1390-1380	s-m	S
				10 ··· 1

TABLE 6.9 Selected In-plane Stretching Vibrations for Selected Pyrroles, Furans and Thiophenes

(Continued)

			Intensities ¹	
Pyridine	Assignment	Region (cm ⁻¹)	IR	R
2-subst pyrrole	Quadrant str.	1570-1545	w-m	m
	Quadrant str.	1475-1460	m	vs
	Semi-circle str.	1420-1400	s-m	s
3-subst pyrrole	Quadrant str.	1570-1560	w-m	m
	Quadrant str.	1490-1480	m	vs
	Semi-circle str.	1430-1420	s-m	s
Furan	=CH str.	3156, 3121, 3092	m	s-m
	Quadrant str. + CH rk	1590	S	W
	Quadrant str. + CH rk	1483	S	vs
	Semi-circle str + CH rk	1378	s	s
	Ring in-phase str.	1138	_	vs
2-subst furan	Quadrant str.	1560-1540	w-m	m
	Quadrant str.	1510-1490	m	vs
	Semi-circle str.	1390-1380	s-m	s
Thiophene	=CH str.	3110, 2998	m	s-m
	Quadrant str. + CH rk	1588	S	-
	Quadrant str. $+$ CH rk	1408	s	vs
	Semi-circle str + CH rk	1357	S	s
	Ring in-phase str.	1031	-	vs
	Quad bend	832	s	vs
2-subst thiophene	Quadrant str.	1540-1514	w-m	m
	Quadrant str.	1455-1430	m	vs
	Semi-circle str.	1361–1345	s-m	S

 TABLE 6.9
 Selected In-plane Stretching Vibrations for Selected Pyrroles, Furans and Thiophenes—cont'd

				Inte	ensities ¹
Group		Assignment	Frequency (cm ⁻¹)	IR	R
C=O	R–CO–H	C =O str.	1740-1720	s	m
	conj-CO-H	C =O str.	1710-1685	S	w
	R-CO-R	C =O str.	1725-1705	S	m
	conj-CO–R	C =O str.	1700-1670	S	m
	conj-CO-conj	C =O str.	1680-1640	S	m
	H–CO–O–R	C =O str.	1725-1720	s	m
	R-CO-O-R	C =O str.	1750-1735	s	m
	Conj-CO-O-R	C =O str.	1735-1715	s	m
	γ lactones	C =O str.	1795-1760	s	m
	R–CO–OH dimer	C =O o.ph. str.	1720-1680	s	-
	"	C =O i.ph. str.	1670-1630	_	m
	R-CO-N	C =O str.	1695-1630	s	m
	R-CO-Cl	C =O str.	1810-1775	s	m
	R-CO-O-CO-R	C =O i.ph. str.	1825-1815	s	m
	"	C =O o.ph. str.	1755-1745	ms	m
	Cyclic anhydride	C =O i.ph. str.	1870-1845	m	s
	" "	C =O o.ph. str.	1800-1775	s	mw
	$R-CO_2^-$	CO ₂ o.ph. str.	1650-1540	s	w
	"	CO ₂ i.ph. str.	1450-1360	ms	s

 TABLE 6.10
 Selected Group Frequencies: Carbonyls

 $^{1}s = strong, m = medium, w = weak, v = very, br = broad, var. = variable, - = zero$

				Inter	nsities ¹
Group		Assignment	Frequency (cm ⁻¹)	IR	R
он	R–OH O	OH str.	3400-3200	sbr	vw
	O=C-OH dimer	OH str.	3200-2600	sbr	
	"	OH wag	960-875	m	11 <u></u>
	Р-ОНО	OH str.	2800-2100	s br	vw
	S-OHO	OH str.	3100-2200	sbr	vw
C-O	CH ₂ -O-CH ₂	COC o.ph. str	1270-1060	S	w
	"	COC i.ph. str.	1140-800	m	s
	C=C-O-CH ₂	COC o.ph. str.	1225-1200	s	w
	Ar–O–CH ₂	Ar–O str.	1310-1210	S	m
	"	O-CH ₂ str.	1050-1010	m	m
	CH ₂ –OH	C–O str.	1090-1000	S	mw
	"	C–O str.	900-800	mw	s

 TABLE 6.11
 Selected Group Frequencies: Alcohols and Ethers

				Inter	nsities ¹
Group		Assignment	Frequency (cm ⁻¹)	IR	R
	R ₂ CH–OH	C–O str.	1150-1075	m	mw
	"	C–O str.	900-800	mw	S
	R ₃ C–OH	C–O str.	1210-1100	S	mw
	"	C–O str.	800-750	mw	S
	Ar–OH	C–O str.	1260-1180	S	w
	O=C-O-C	C–O str.	1300-1140	S	w
	О=С-ОН	C–O str.	1300-1200	S	W
	Ероху	ring i.ph. str.	1270-1245	m	S
	"	ring o.ph. str.	935-880	s	m
	11	ring o.ph. str.	880-830	S	m

 TABLE 6.11
 Selected Group Frequencies: Alcohols and Ethers—cont'd

s = strong, m = medium, w = weak, v = very, br = broad, var. = variable, - = zero

			Intensities ¹	
Group	Assignment	Frequency (cm ⁻¹)	IR	R
CH ₂ -NH ₂	NH ₂ o.ph. str.	3500-3300	m	vw
ш	NH ₂ i.ph. str.	3400-3200	m	m
	NH ₂ bend	1630-1590	m	vw
	NH ₂ wag	900-600	sbr	W
CH ₂ -NH-CH ₂	NH str.	3450-3250	vw	w
S.M.	C–N–C o.ph. str.	1150-1125	m	mw
Ar–NH ₂	C–N str.	1380-1260	sbr	m
C-NH ₃ ⁺ X ⁻	NH ₃ str.	3200-2700	S	vw
	NH ₃ o.ph. bend	1625-1560	mw	vw
."	NH ₃ i.ph. bend	1550-1505	w	vw

 TABLE 6.12
 Selected Group Frequencies: Nitrogen Compounds

			Intensities ¹	
Group	Assignment	Frequency (cm ⁻¹)	IR	R
$C_2NH_2^{+\dots}X^-$	NH ₂ str.	3000-2700	sbr	w
"	NH ₂ bend	1620-1560	mw	w
$C_3 NH^{+\dots} X^{-}$	NH str.	2700-2300	S	w
$O = C - NH_2$	NH ₂ o.ph. str.	3475-3350	s	w
"	NH ₂ i.ph. str.	3385-3180	S	w
"	NH ₂ bend	1650-1620	ms	w
O =C-NH-C	NH str.	3320-3270	ms	w
"	CNH str. bend	1570-1515	ms	w
O =C-NH-C cyclic	NH str.	3300-3100	ms	w
>C = N	C = N str	1690-1630	mw	ms
>C = N - OH	OH str.	3300-3150	s	w
"	N–O str.	1000-900	S	S
CH ₂ -NO ₂	NO ₂ o.ph. str.	1600-1530	s	mw
"	NO ₂ i.ph. str.	1380-1310	s	vs
Ar-NO ₂	NO ₂ o.ph. str.	1555-1485	s	_
"	NO ₂ i.ph. str.	1357-1318	S	vs
C-O-NO ₂	NO ₂ o.ph. str.	1640-1620	S	mw
"	NO ₂ i. ph. str.	1285-1220	S	S
11	N–O str.	870-840	s	S
С-О-N=О	s-trans N =O str.	1681-1640	S	S
"	<i>s</i> -cis N =O str.	1625-1600	S	S

 TABLE 6.12
 Selected Group Frequencies: Nitrogen Compounds—cont'd

s = strong, m = medium, w = weak, v = very, br = broad, var. = variable, - = zero

			Intensities ¹	
Group	Assignment	Frequency (cm ⁻¹)	IR	R
CF ₂ and CF ₃	CF str.	1350-1120	vs	mw
Ar-F	CF str.	1270–1 <mark>100</mark>	S	m
C–Cl	C–Cl str.	830-560	S	s
C-CH ₂ -CH ₂ -Cl	trans C-Cl str.	730-720	s	S
11	gauche C–Cl str.	660-650	S	S
CH ₂ –Cl	CH ₂ wag	1300-1240	s	S
C-Br	C–Br str.	700-515	S	VS
C-CH ₂ -CH ₂ -Br	trans C-Br str.	650-640	s	vs
Ш	gauche C–Br str.	565-560	S	vs
CH ₂ –Br	CH ₂ wag	1250-1220	s	m

 TABLE 6.13
 Selected Group Frequencies: Halogen Compounds

s = strong, m = medium, w = weak, v = very, br = broad, var. = variable, - = zero.

				Inte	nsities ¹
Group		Assignment	Frequency (cm ⁻¹)	IR	R
Sulfur Cpds	SH	SH str.	2590-2540	w	s
	C-SO ₂ -C	SO ₂ o.ph. str.	1340-1290	s	w
	"	SO ₂ i.ph. str.	1165-1120	s	s
	C-SO ₂ -N	SO ₂ o.ph. str.	1380-1310	s	m
	"	SO ₂ i.ph. str.	1180-1140	s	s
	C-SO ₂ -O-C	SO ₂ o.ph. str.	1375-1335	s	ms
	"	SO ₂ i.ph. str.	1195-1165	s	s
	C–SO ₂ –Cl	SO ₂ o.ph. str.	1390-1361	S	w
	"	SO ₂ i.ph. str.	1181-1168	s	s
	C–SO ₂ –OH anhydrous	OH str.	3100-2200	sbr	w
		SO ₂ o.ph. str.	1352-1342	s	w
		SO ₂ i.ph. str.	1165-1150	s	s
	$C-SO_3^-$ H ₃ O ⁺ (hydrate)	OH str.	2800-2100	sbr	_
		SO3 o.ph. str.	1230-1120	s	_
		SO3 i.ph. str.	1085-1025	m	_
	$C_2S = O$	S =O str.	1065-1030	s	w
Phosphorus Cpds	PH	PH str.	2450-2270	ms	mw
	P=O	P =O str.	$1320 - 1140^2$	s	m
	Р-ОН	OH str.	2800-2100	sbr.	vw
	P-O-CH ₂	P–O–C str.	1050-970	s	mw
	P–O–Ar	O–Ar str.	1240-1160	S	mw
	"	P–O str.	995-855	s	w
Silicon Cpds	SiH	Si–H str.	2250-2100	vs	m
	Si-O	Si–O str.	1100-1000	vs	w
	Si-CH ₃	CH3 i.ph. bend	1270-1250	vs	w

 TABLE 6.14
 Selected Group Frequencies: Sulfur, Phosphorus, Silicon, and Boron Compounds

(Continued)

				Intensities ¹	
Group		Assignment	Frequency (cm ⁻¹)	IR	R
Boron Cpds	BH	B–H str	2640-2350	s	mw
	BH (complete octet)	B–H str	2400-2200	s	mw
	B–H–B (Bridge)	B–H–B str.	2220-1540	s	mw
	В-ОН	OH str	3300-3200	s	W
	В-О	B–O str	1380-1310	s	var
	B-N	B–N str.	1465-1330	s	var
	B-Phenyl	C–B–C/ring str.	1440-1430	s	

TABLE 6.14 Selected Group Frequencies: Sulfur, Phosphorus, Silicon, and Boron Compounds-cont'd

 $^{1}s = strong, m = medium, w = weak, v = very, br = broad, var. = variable, - = zero$ $^{2}Electronegative substituents raise the P = O frequency (example: R_3P = O ~ 1160 cm⁻¹, (R-O)_3P = O ~ 1270 cm⁻¹)$

INORGANICS

Inorganics	IR bands (cm ⁻¹)	Raman bands (cm ⁻¹)
NH4 ⁺	3100 s, 1410 s	3100 w, 1410 w
NCO ⁻	2170 vs, 1300 m, 1210 m	2170 m, 1300 s, 1260 s
NCS ⁻	2060 vs	2060 s
CN^{-}	2100 m	2080 s
CO ₃ ⁻	1450 vs, 880 m, 710 w	1065 s
HCO ₃ ⁻	1650 m, 1320 vs	1270 m, 1030 s
NO ₃ ⁻	1390 vs, 830 m, 720 w	1040 s
NO_2^-	1270 vs, 820 w	1320 s
$\mathrm{SO_4}^{-2}$	1130 vs, 620 m	980 s
HSO_4^-	1240 vs, 1040 m, 870 m	1040 s, 870 m
SO ₃ ⁻	980 vs	980 s
PO_4^{-3}	1030 vs, 570 m	940 s
$(-\mathrm{SiO}_2^-)_x$	1100 vs, 470 m	_
TiO ₂	660 vs, 540 vs	_

 TABLE 6.15
 Selected Group Frequencies: Common Inorganic Compounds

s = strong, m = medium, w = weak, v = very, - = zero.