Third Edition

A. D. CROSS and
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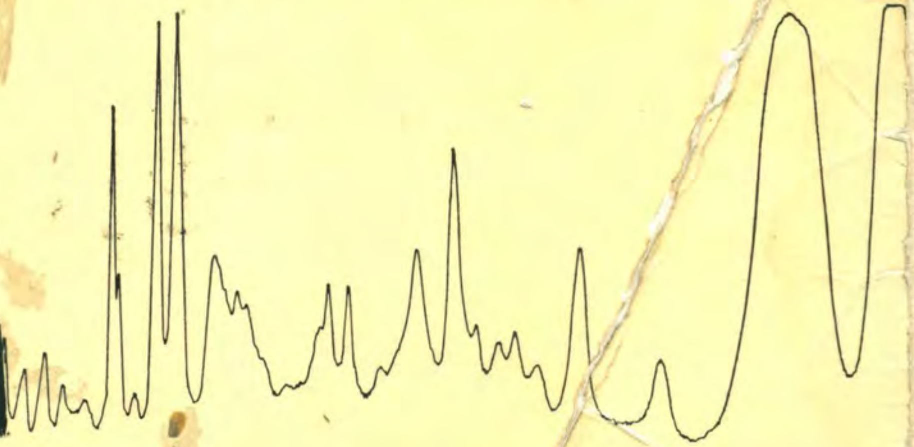
An Introduction to
PRACTICAL INFRA-RED SPECTROSCOPY



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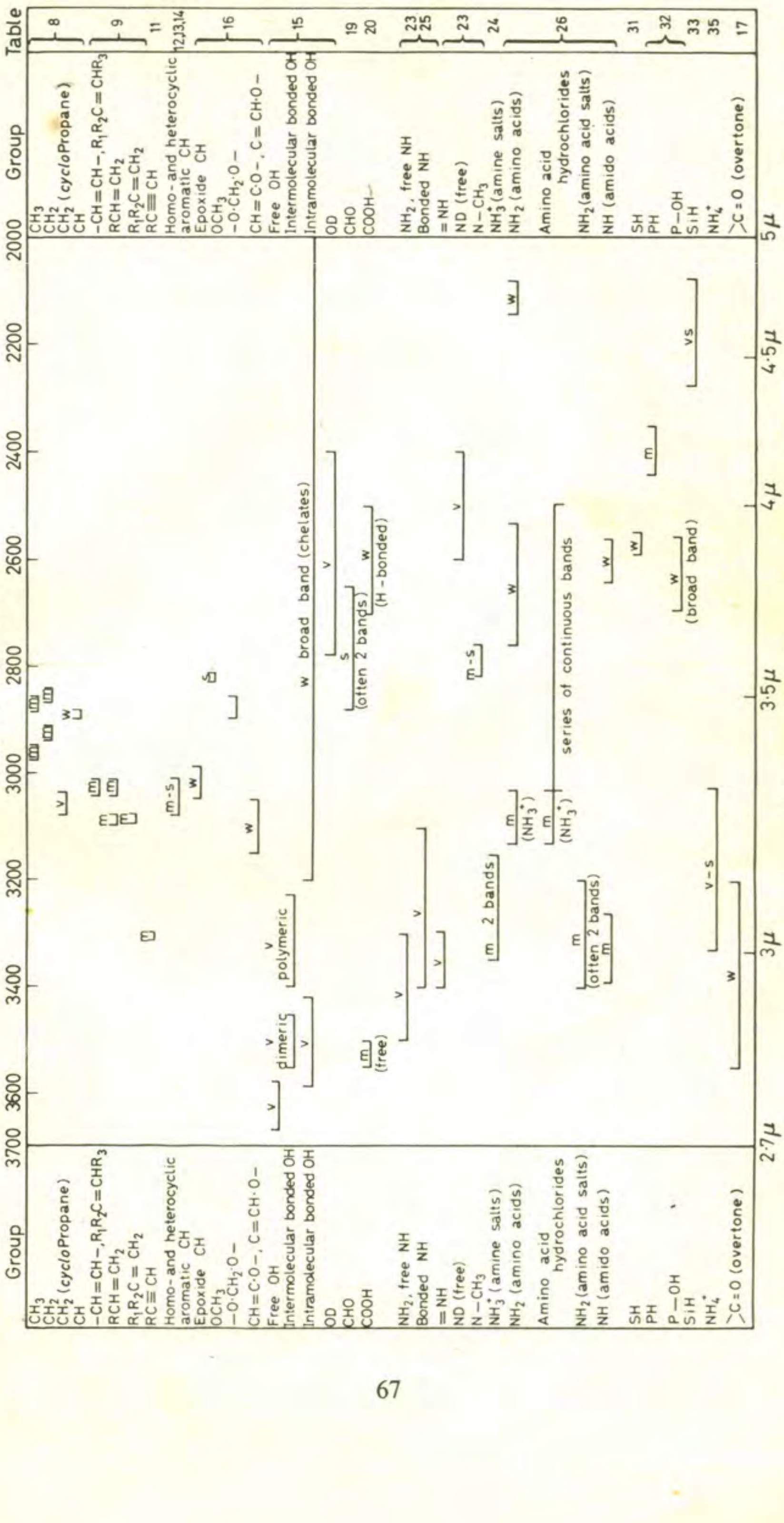
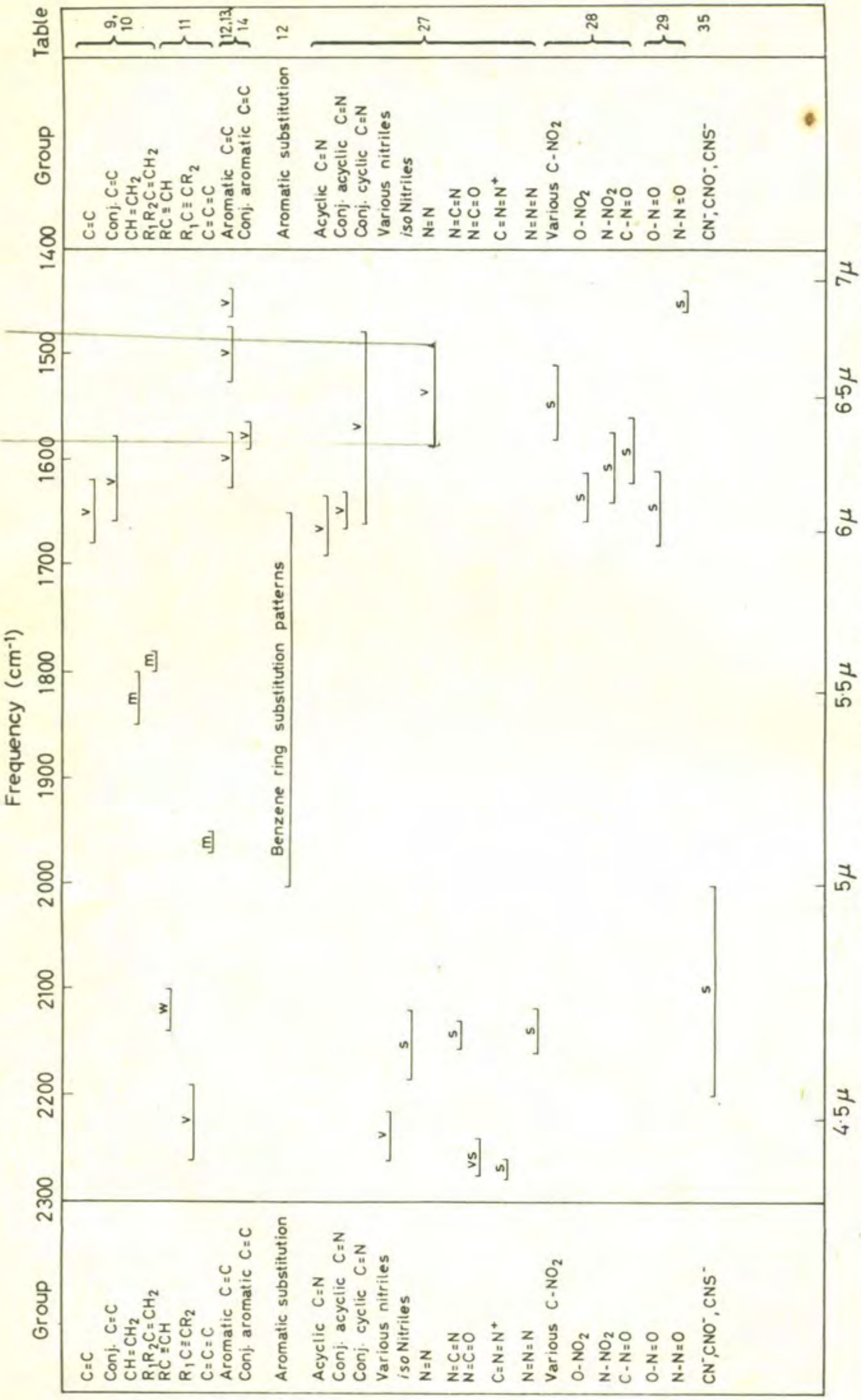
ABBREVIATIONS

adj.	adjacent	s.	strong intensity
approx.	approximately	sat.	saturated
asym.	asymmetrical	sec.	secondary
conj.	conjugated	soln.	solution
def.	deformation	so. ph.	solid phase
dil.	dilute	spec.	spectrum
enh.	enhanced	str.	stretching
i.b.	inconsistent band	sym.	symmetrical
int.	intensity	tert.	tertiary
i.p.	in-plane	unsat.	unsaturated
liq. ph.	liquid phase	v.	variable intensity
l.v.	limited value assignment	vap. ph.	vapour phase
m.	medium intensity	vib.	vibration
non-conj.	non-conjugated	v.s.	very strong intensity
o.o.p.	out-of-plane	w.	weak intensity
'5' ring	5-membered ring, etc.		



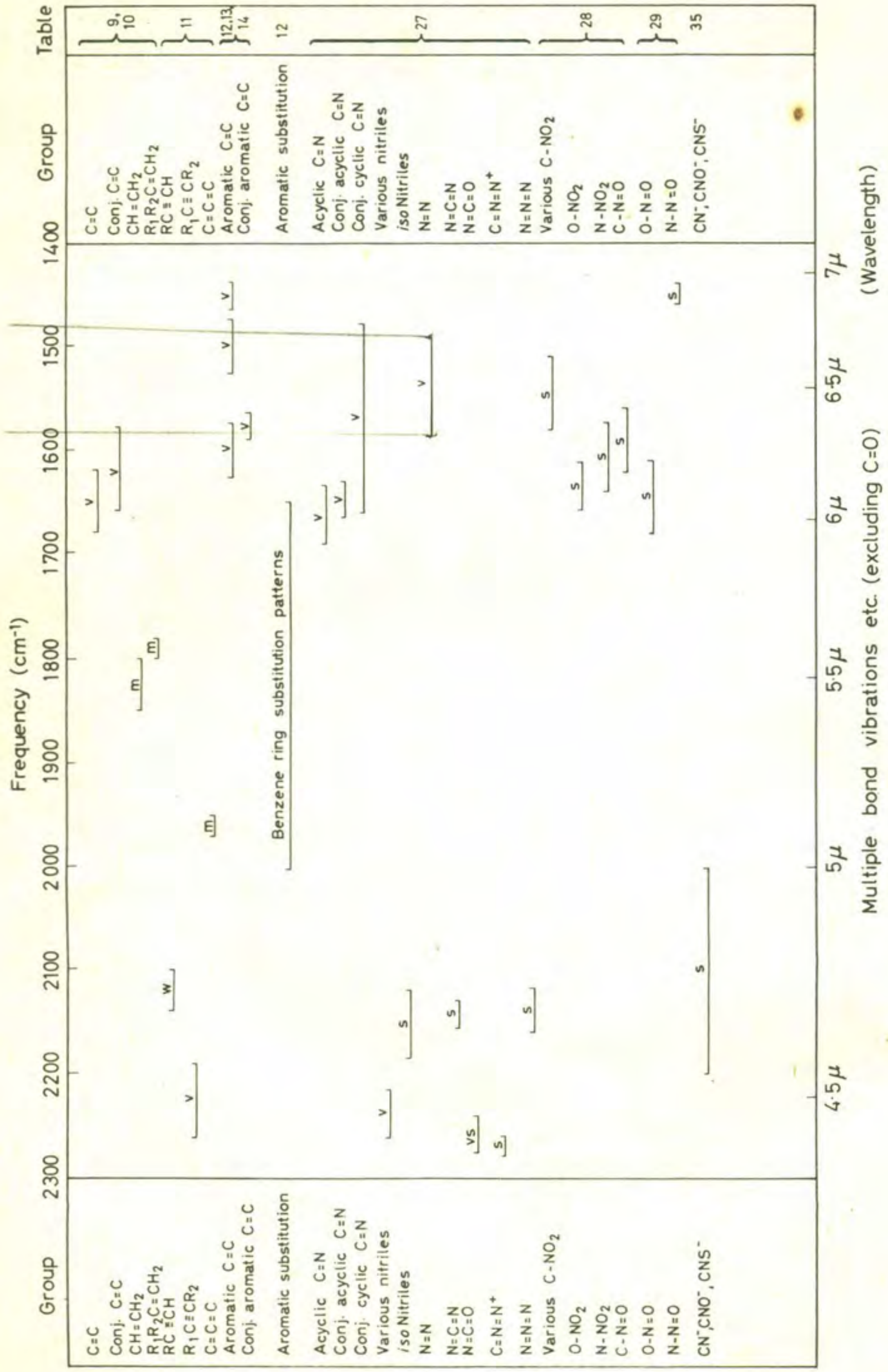
Hydrogen stretching vibrations etc.

Correlation Chart I

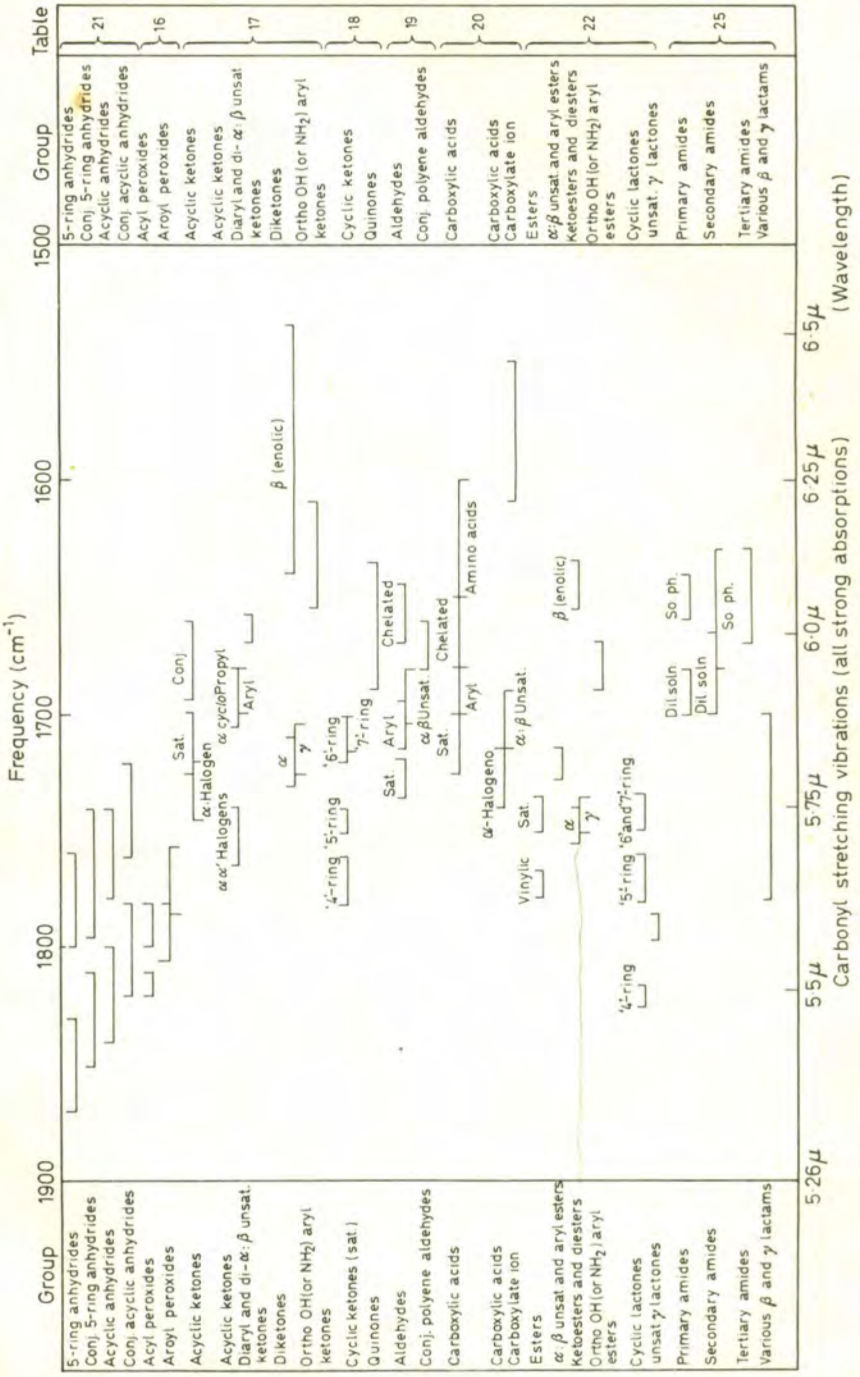


Multiple bond vibrations etc. (excluding C=O)

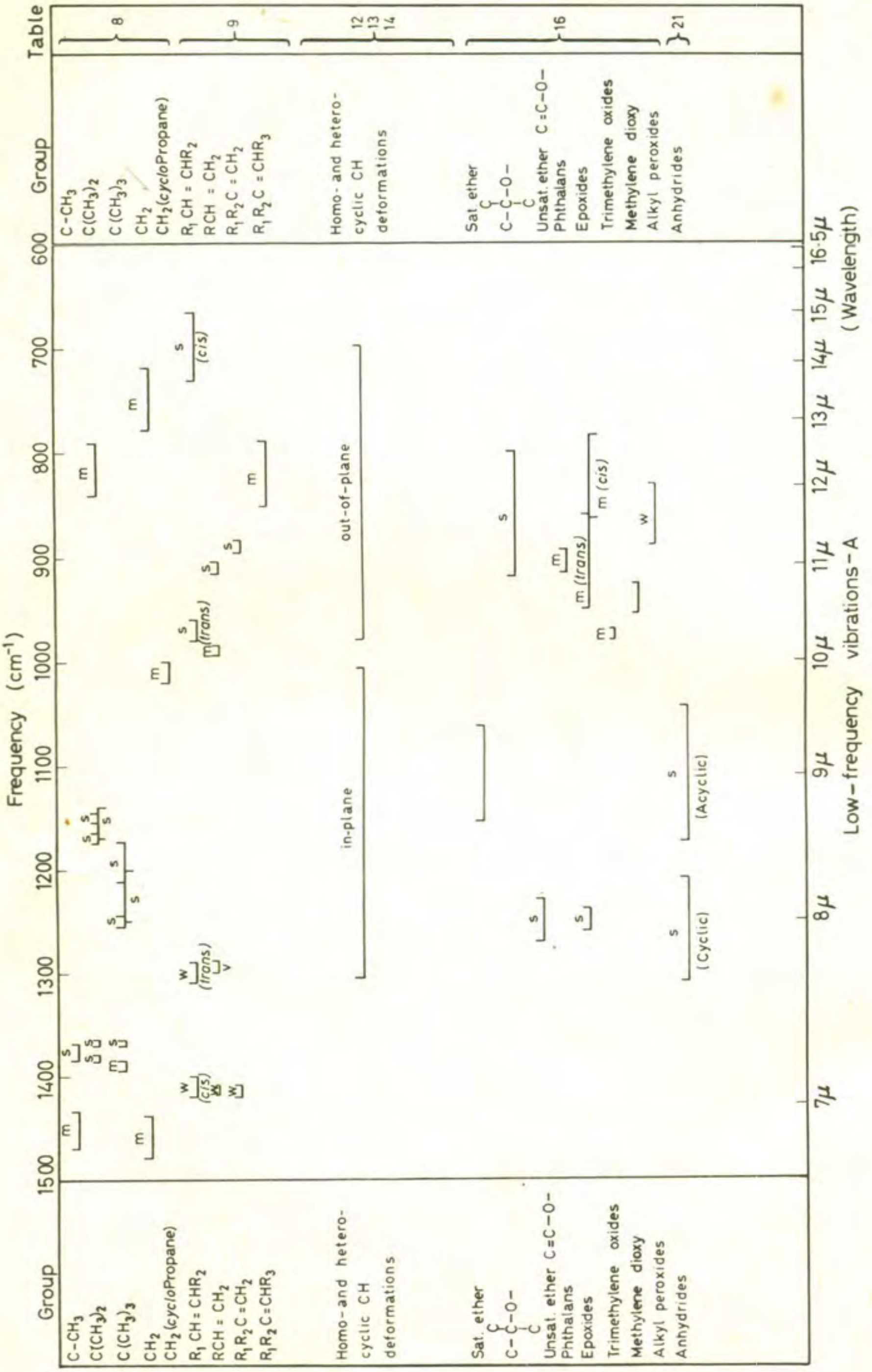
Correlation Chart II



Correlation Chart II

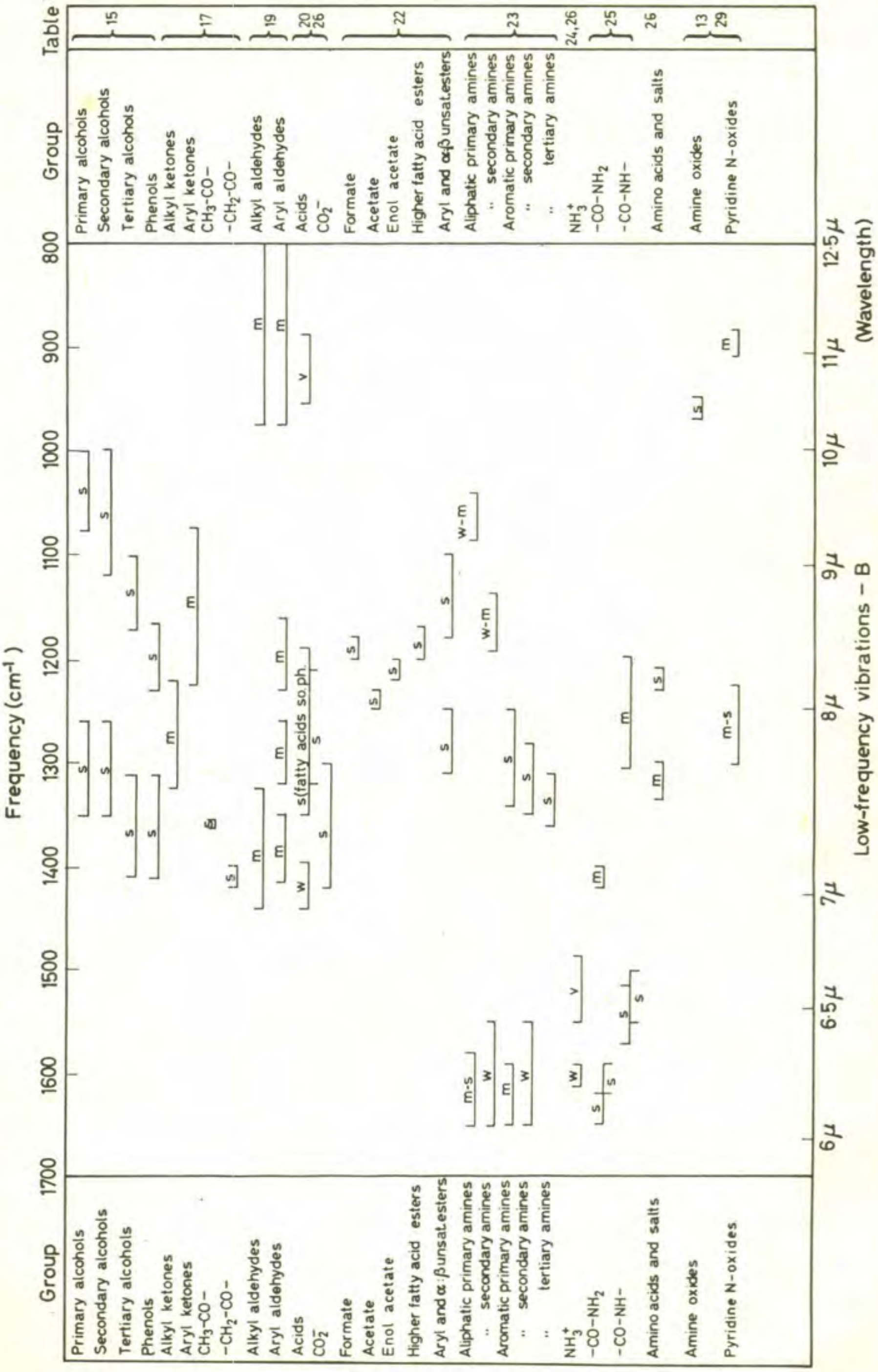


Correlation Chart III



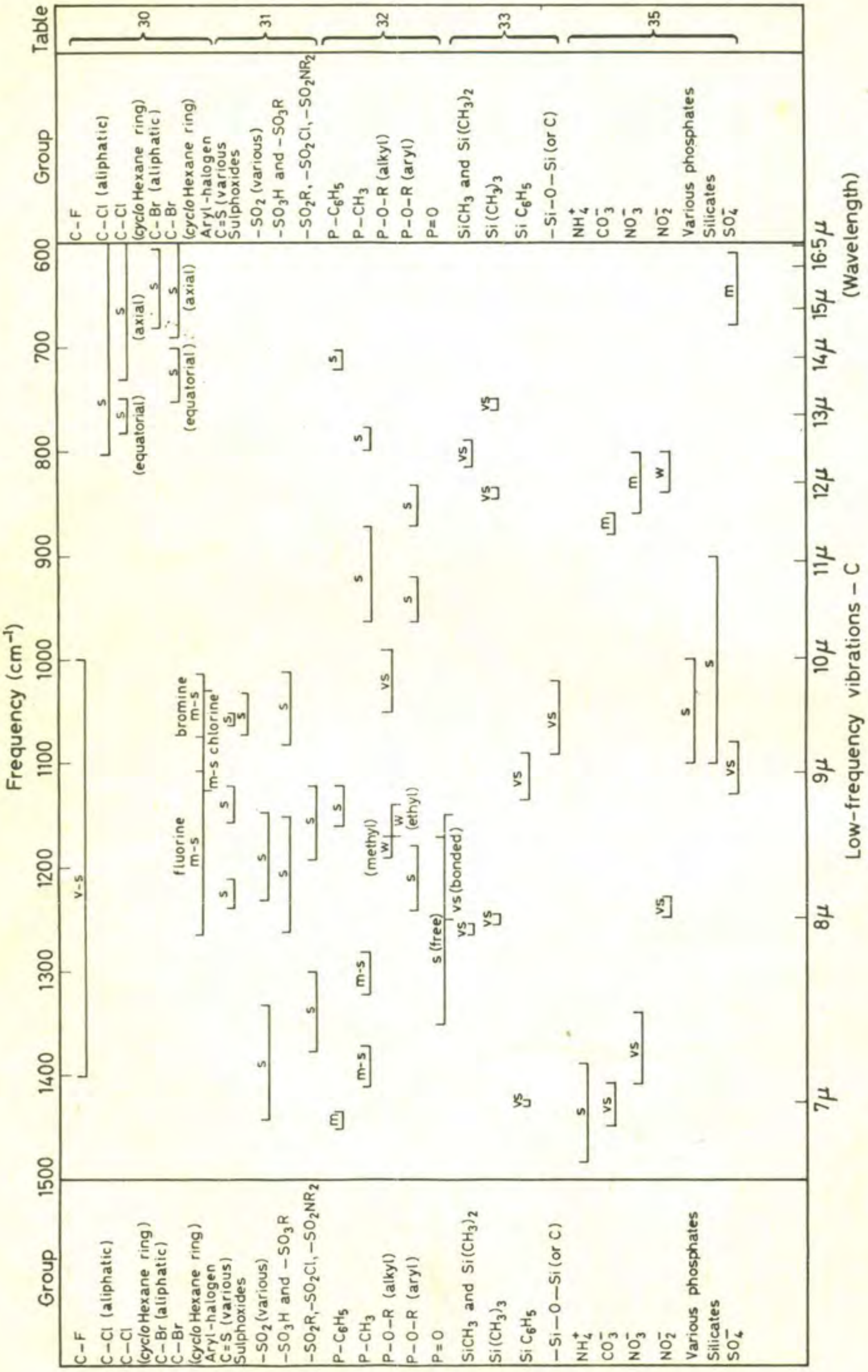
Low-frequency vibrations–A

Correlation Chart IV



Low-frequency vibrations – B

Correlation Chart V



Correlation Chart VI

For boron compounds and many inorganic ions the tables should be consulted.

ALKANES

Table 8. Alkanes and Cycloalkanes*

C—H *Stretching Vibrations*

Alkyl—CH_3	2,975–2,950	3·36–3·39	m.	The presence of several of these groups gives strong absorption.
	2,885–2,860	3·47–3·50	m.	
Aryl—CH_3	2,930–2,920	3·41–3·43	m.	
	2,870–2,860	3·48–3·50	m.	
acyclic—CH_2—	2,940–2,915	3·40–3·45	m.	
	2,870–2,845	3·49–3·52	m.	
acyclic—CH—	2,900–2,880	3·45–3·47	w.	
*cyclo*propanes	3,100–3,070	3·23–3·26	v.	
	3,030–2,995	3·30–3·34	v.	
*cyclo*butanes	2,990–2,980	3·34–3·36	v.	
	2,925–2,875	3·42–3·48	v.	
*cyclo*pentanes	2,960–2,950	3·38–3·39	v.	
	2,870–2,850	3·48–3·51	v.	
*cyclo*hexanes	2,940–2,910	3·40–3·44	v.	
	2,870–2,840	3·49–3·52	v.	

C—H *Deformation Vibrations*

C—CH_3	1,470–1,435	6·80–6·97	m.	asym. def.
	1,385–1,370	7·22–7·30	s.	sym. def.
$C(CH_3)_2$	1,385–1,380	7·22–7·25	s.	doublet of approx. equal int.
	1,370–1,365	7·30–7·33	s.	
$C(CH_3)_3$	1,400–1,390	7·14–7·19	m.	doublet int. ratio *ca.* 1:2
	1,375–1,365	7·27–7·33	s.	
—CH_2—	1,480–1,440	6·76–6·94	m.	CH_2 scissor
—CH—	*ca.* 1,340	*ca.* 7·46	w.	l.v.

Skeletal Vibrations

$C(CH_3)_2$	1,175–1,165	8·51– 8·58	s.	
	1,150–1,130	8·90– 8·85	s.	
	840– 790	11·90–12·66	m.	l.v.
$C(CH_3)_3$	1,255–1,245	7·97– 8·03	s.	
	1,210–1,160	8·26– 8·62	s.	
acyclic—$(CH_2)_n$—				
n = 4 or more	725– 720	13·79–13·89	m.	
n = 3	730– 725	13·70–13·79	m.	
n = 2	740– 735	13·51–13·65	m.	
n = 1	785– 770	12·74–12·99	m.	
*cyclo*propane	1,050–1,000	9·52–10·00	m.	l.v.

* For absorption due to OCH_3, NCH_3, etc. see ethers, amines, etc.

ALKENES, ALKYNES, AND ALLENES

Table 9. Alkenes

$C=C$ *Stretching Vibrations*

non-conj. $C=C$	1,680–1,620	5·95–6·17	v.	
$CHR=CH_2$	1,645–1,640	6·08–6·10	v.	
$CHR_1=CHR_2$ (*cis*)	1,665–1,635	6·01–6·12	v.	
$CHR_1=CHR_2$ (*trans*)	1,675–1,665	5·97–6·00	v.	
$CR_1R_2=CH_2$	1,660–1,640	6·02–6·10	v.	
$CR_1R_2=CHR_3$	1,690–1,670	5·92–5·99	v.	
$CR_1R_2=CR_3R_4$	1,690–1,670	5·92–5·99	w.	l.v.
aryl—$C=C$	*ca.* 1,625	*ca.* 6·16	s.	enh. int.
$C=C·C=O$ or $C=C·C=C$	1,660–1,580	6·02–6·33	s.	cisoid form int. often more enh. than transoid

C—H *Stretching and Deformation Vibrations*

$CHR_1=CH_2$	3,040–3,010	3·29– 3·32	m.	CH str. (CHR_1)
	3,095–3,075	3·23– 3·25	m.	CH str. (CH_2)
	995– 985	10·05–10·15	m.	CH o.o.p. def.
	915– 905	10·93–11·05	s.	CH_2 o.o.p. def.
	1,850–1,800	5·41– 5·56	m.	overtone
	1,420–1,410	7·04– 7·09	w.	CH_2 i.p. def.
	1,300–1,290	7·69– 7·75	v.	CH i.p. def.
$CHR_1=CHR_2$ (*cis*)	3,050–3,000	3·28– 3·33	m.	CH str.
	1,420–1,400	7·04– 7·14	w.	CH i.p. def.
	730– 665	13·70–15·04	s.	CH o.o.p. def.
$CHR_1=CHR_2$ (*trans*)	3,050–3,000	3·28– 3·33	m.	CH str.
	980– 960	10·20–10·42	s.	CH o.o.p. def.
	1,310–1,290	7·63– 7·75	w.	CH i.p. def.
$CR_1R_2=CH_2$	3,095–3,075	3·23– 3·25	m.	CH str.
	895– 885	11·17–11·30	s.	o.o.p. def.
	1,800–1,780	5·56– 5·62	m.	overtone
	1,420–1,410	7·04– 7·09	w.	CH_2 i.p. def.
$CR_1R_2=CHR_3$	3,040–3,010	3·29– 3·32	m.	CH str.
	850– 790	11·76–12·66	m.	CH o.o.p. def.

The $C=C$ stretching frequency is affected by both the mesomeric and inductive effects of substituents attached directly to the double bond. The $=CH_2$ out of plane deformation of the vinyl group is sensitive only to the mesomeric effect, whereas the $CH=CH$ trans CH deformation is relatively insensitive to the mesomeric effect but is affected by the inductive effects.

	$C=C$ str.	$=CH_2$ o.o.p. def.	$CH=CH$ def.
$CH_2=CHR$	*ca.* 1,640	*ca.* 910	*ca.* 990
$CH_2=CHCO.OR$	1,640–1,630	*ca.* 961	*ca.* 982
$CH_2=CHO.CO.R$	1,700–1,665	*ca.* 870	*ca.* 950
$CH_2=CHOR$	1,680–1,660	*ca.* 815	*ca.* 960
$CH_2=CHF$	*ca.* 1,650	*ca.* 860	*ca.* 925
$CH_2=CF_2$	1,755–1,735	*ca.* 800	—

During vibrations of the $C=C$ and $C=O$ groups of acyclic alkenes and ketones the carbon atoms directly attached to the multiple bond usually remain stationary, thereby localizing the vibration within the bond. However, the observed stretching frequency of the C=C bond of cyclic alkenes represents a coupled vibration of the C=C stretching mode with the stretching and bending modes of the adjacent C—C bond and therefore varies with the size of the ring. The minimum interaction occurs at a C=C—C angle of 90° when the C=C stretching vibration causes only bending of the attached C—C bond. At higher or lower angles C—C stretching also occurs as a result of the C=C stretching vibration. This increase in vibrational interaction produces an increase in the C=C stretching frequency. In acyclic systems the bond angles are usually invariant at *ca.* 120° and the interaction and consequently the position of the absorption band are fairly constant. For the cyclic compounds the wavelength of the C=C stretching vibration is directly related to $\cos^2\alpha$, where α is the C=C—C angle[5]. Hence, although the ring strain in cyclopropene and cyclohexene differ considerably, the positions of the observed C=C stretching bands are almost identical. Such a coincidence in the values would not have been predicted if the change in the stretching frequency was entirely dependent upon a change in the force constants, resulting from a rehybridization of the sp^2 orbitals[6].

Alkyl substitution of the alkene bond increases the C=C stretching frequency as further interaction can occur between the double bond and the C-alkyl bond, e.g. cyclopropene absorbs at 1,640 (6·10), 1,3,3,-trimethylcyclopropene at 1,765 (5·70), and 1,2,3,3,-tetramethylcyclopropene at 1,865 cm^{-1} (5·36 μ).

Similar arguments explain the increase in the frequencies of the C=O and C=C stretching vibrations of cyclic ketones (*Table 18*) and exocyclic alkenes with a decrease in the size of the rings.

Table 10. Cyclic and Exocyclic Alkenes

C—H *and* C=C *Stretching Vibrations*					
*cyclo*propenes	*ca.* 3,080	*ca.* 3·25	*cyclo*heptenes	*ca.* 1,650	*ca.* 6·06
	ca. 1,640	*ca.* 6·10	*cyclo*octenes	*ca.* 1,675	*ca.* 5·97
*cyclo*butenes	*ca.* 3,060	*ca.* 3·27	exocyclic alkenes,		
	ca. 1,565	*ca.* 6·39	$(CH_2)_nC=CH_2$		
*cyclo*pentenes	*ca.* 3,040	*ca.* 3·29	n = 2	*ca.* 1,780	*ca.* 5·62
	ca. 1,610	*ca.* 6·21	n = 3	*ca.* 1,680	*ca.* 5·95
*cyclo*hexenes	*ca.* 3,010	*ca.* 3·32	n = 4	*ca.* 1,660	*ca.* 6·02
	ca. 1,645	*ca.* 6·08	n = 5	*ca.* 1,650	*ca.* 6·06

Table 11. Alkynes and Allenes

Alkynes				
$RC\equiv CH$	3,340–3,300	2·99–3·03	m.	C—H str.
	2,140–2,100	4·67–4·76	w.	C≡C str.
$R_1C\equiv CR_2$	2,260–2,190	4·43–4·57	v.	C≡C str.
Allenes				
C=C=C	2,000–1;900	5·00–5·26	m.-s.	asym. CCC str.
	ca. 850	*ca.* 11·76	s.	CH_2 o.o.p. def.

AROMATIC HOMOCYCLIC AND HETEROCYCLIC COMPOUNDS

Table 12. Aromatic Homocyclic Compounds

Stretching Vibrations

$=$C—H str.	3,100–3,000	3·25–3·33	w.-m.	multiple peaks may appear in this region
C$=$C i.p. def	1,625–1,590	6·15–6·29	v.	usually close to 1,600 cm^{-1}
	1,590–1,570	6·29–6·37	v.	
	1,520–1,470	6·58–6·80	v.	usually close to 1,500 cm^{-1}
	1,465–1,430	6·83–6·99	v.	

Attempts have been made to rationalize the wide variations in the intensities of the ring vibrations in the 1,600–1,400 cm^{-1} region. It has been found that there is a general increase in the intensity of the bands, particularly of those near 1,600 cm^{-1}, as a result of charge disturbance within the ring through the electronic interaction between the ring and the substituents. More recent studies have correlated the square root of the integrated intensities of these bands with the σ_R^0 factors for the substituents[7]. The intensity of the 1,580 cm^{-1} band is considerably enhanced when the ring is conjugated with a carbonyl group.

The bands at 1,010, 992, and 606 cm^{-1} for unsubstituted benzene result from in-plane C—C deformation modes in which the carbon atoms move

C—H *In-plane Deformations and Benzene Ring Substitution*

monosubstitution	1,250–1,230	8·00–8·13	w.
	1,180–1,170	8·48–8·55	w.-m.
	1,160–1,150	8·62–8·70	w.
	1,080–1,065	9·26–9·39	m.
	1,030–1,025	9·71–9·76	w.-m.
1:2 disubstitution	1,290–1,250	7·75–8·00	w.
	1,180–1,150	8·48–8·70	w.-m.
	1,150–1,100	8·70–9·09	w.-m.
	1,055–1,010	9·48–9·90	m.
1:3 disubstitution	1,300–1,260	7·69–7·94	w.
	1,165–1,150	8·59–8·70	v.
	1,120–1,085	8·93–9·22	w.
	1,090–1,060	9·17–9·43	v.
1:4 disubstitution	1,300–1,265	7·69–7·91	w.-m.
	1,190–1,155	8·40–8·66	v.
	1,130–1,100	8·85–9·09	v.
	1,025–1,000	9·76–10·00	v.
1:2:3 trisubstitution	1,165–1,555	8·59–8·66	w.
	1,085–1,065	9·22–9·39	m.
	1,025–1,010	9·76–9·90	m.
1:2:4 trisubstitution	1,160–1,140	8·62–8·77	m.
	1,140–1,120	8·77–8·93	m.
	1,045–1,025	9·57–9·76	m.
1:3:5 trisubstitution	1,180–1,160	8·48–8·62	m.

radially or nearly so. For substituted benzenes these 'radial modes' can interact with the single bond stretching vibration of the attached substituent. Consequently these vibrations will be sensitive to the mass of the substituent. These bands have been termed 'X-sensitive bands'[8] and, in some instances, they can be used to characterize the X-substituent. Where this is so, mention of the band, which is usually to be found in the 1,300–1,050 cm^{-1} region, has been made in the relevant Tables.

In the case of monosubstituted and *meta*-disubstituted benzenes a 'radial mode' in which the carbon atoms 2, 4 and 6 move radially in phase and is therefore virtually insensitive to the mass of the substituent, is observed near 1,000 cm^{-1}. This vibration is called the ring breathing mode.

X-sensitive mode

Ring breathing mode

C—H *Out-of-plane Deformations and Benzene Ring Substitution*

monosubstitution	900–860	11·11–11·63	w.-m.	5 adj. H atoms, l.v.
	770–730	12·99–13·70	s.	5 adj. H atoms
	710–690	14·08–14·49	s.	5 adj. H atoms
✓1:2 disubstitution	960–905	10·42–11·05	w.	4 adj. H atoms, l.v.
	850–810	11·76–12·35	w.	4 adj. H atoms, l.v.
	760–745	13·16–13·42	s.	4 adj. H atoms
1:3 disubstitution	960–900	10·42–11·11	m.	isolated H atom
	880–830	11·36–12·05	m.-s.	3 adj. H atoms
	820–790	12·20–12·66	w.-m.	3 adj. H atoms, l.v.
1:4 and 1:2:3:4 substitution	860–800 645	11·63–12·50	s.	2 adj. H atoms
1:2:3 trisubstitution	965–950	10·36–10·53	w.	3 adj. H atoms, l.v.
	900–885	11·11–11·30	w.	3 adj. H atoms, l.v.
	780–760	12·82–13·16	s.	3 adj. H atoms
	720–685	13·89–14·60	m.	3 adj. H atoms, l.v.
1:2:4 trisubstitution	940–920	10·64–10·87	w.	isolated H atom, l.v.
	900–885	11·36–11·30	m.	2 adj. H atoms
	780–760	12·82–13·16	s.	2 adj. H atoms
1:3:5 trisubstitution	950–925	10·53–10·81	v.	isolated H atom, l.v.
	860–830	11·49–12·05	s.	isolated H atom
1:2:3:5, 1:2:4:5, and 1:2:3:4:5 substitution	870–850	11·49–11·76	s.	isolated H atom

Benzene Ring Substitution Patterns of Summation Bands

Weak summation bands (overtones and combinations) of the CH out-of-plane deformation frequencies give absorption patterns in the range 2,000–1,650 cm^{-1} (5·00–6·06 μ), which are consistent and characteristic of the different substitutions of the benzene ring. Strong solutions are required to study these patterns [up to 20 times normal solution strengths (p. 23)]. Other bands occurring in this region, e.g. the strong C=C and C=O stretching fundamentals, mask the aromatic bands. Since the number of bands, their intensities and band shapes are more characteristic than absolute frequencies, no table is included here. These patterns are very useful in structural analysis and, though reference patterns are available[9], a preferred procedure is to prepare a set for each individual instrument.

Polycyclic Aromatic Compounds

Condensed ring systems absorb in similar regions to those observed for monocyclic aromatic compounds and, in general, the hydrogen substitution pattern for each ring may be considered separately. Thus, naphthalenes have two bands near 1,600 cm^{-1} (6·25) and bands in the ranges 1,520–1,505 (6·58–6·65) and 1,400–1,390 cm^{-1} (7·14–7·19 μ). 1-Substituted naphthalenes absorb in the regions 810–785 (12·35–12·74) and 780–760 cm^{-1} (12·82–13·16 μ) characteristic of three and four adjacent hydrogen atoms respectively, whilst 2-substituted naphthalenes absorb at 860–835 (11·63–11·98) (an isolated H atom), 835–805 (11·98–12·42) (two adjacent H atoms), and 760–735 cm^{-1} (13·16–13·61 μ) (four adjacent H atoms).

Anthracenes absorb in the range 1,640–1,620 (6·10–6·17) and near 1,550 cm^{-1} (6·45 μ) and may be differentiated from phenanthrenes which have two bands near 1,600 cm^{-1} (6·25 μ) and another band near 1,500 cm^{-1} (6·67 μ).

Table 13. Aromatic Heterocyclic Components: Six-membered Rings*

Pyridines and Related Compounds

Stretching Vibrations				
Pyridines				
=C—H str.	3,095–3,010	3·23– 3·32	m.-s.	multiple peaks
C=C i.p. vib.	1,615–1,575	6·19– 6·35	v.	
	1,590–1,555	6·29– 6·43	v.	
	1,520–1,465	6·58– 6·83	v.	
	1,450–1,410	6·90– 7·09	v.	
	1,000– 990	10·00–10·10	m.	ring breathing vib.
Pyridinium Salts				
N^{+}—H str. (free)	3,340–3,210	2·99– 3·12	v.	multiple bands
(H bonded ion pair)	3,300–2,375	3·03– 4·21	v.	multiple bands
Pyridine 1-oxides				
=C—H str.	3,095–3,010	3·23– 3·32	m.-s.	multiple bands
C=C i.p. vib.	1,645–1,600	6·08– 6·25	v.	
	1,580–1,560	6·33– 6·41	v.	
	1,540–1,475	6·49– 6·78	v.	
	1,450–1,425	6·90– 7·02	v.	
	ca. 1,015	*ca.* 9·85	s.	ring breathing vib. 3-subst. only
N^{+}—O^{-} str.	1,310–1,220	7·64– 8·20	s.	

* For a comprehensive survey and discussion of the spectra of heteroaromatic compounds, see reference 10. Characteristic substitution patterns in the region 2,000 – 1,650 cm^{-1} (5.00 – 6.06μ) have been observed for pyridines[11] and 2,2-bipyridyls[12]

Table 13—continued

C—H *In- and Out-of-plane Deformations and Ring Substitution*

2-monosubstitution	1,295–1,265	7·72– 7·90	w.	pyridines only
	1,150–1,145	8·70– 8·73	w.	pyridines and 1-oxides
	1,115–1,090	8·97– 9·17	w.	pyridines and 1-oxides
	1,055–1,040	9·48– 9·61	w.	pyridines and 1-oxides
	990– 960	10·10–10·42	m.	pyridine 1-oxides only
	780– 740	12·82–13·51	s.	pyridines only
3-monosubstitution	1,200–1,180	8·33– 8·48	v.	pyridines only
	1,160–1,155	8·62– 8·66	v.	pyridine 1-oxides only
	1,130–1,120	8·85– 8·93	w.	pyridines only
	1,120–1,080	8·93– 9·26	w.-m.	pyridine 1-oxides only
	1,110–1,100	9·01– 9·09	w.	pyridines only
	1,045–1,030	9·57– 9·71	w.	pyridines only
	980– 930	10·20–10·75	s.	pyridine 1-oxides only
	920– 890	10·87–11·24	w.	pyridines only
	820– 770	12·20–12·29	m.-s.	pyridines and 1-oxides
	730– 690	13·70–14·49		pyridines only
	680– 660	14·71–15·15	m.	pyridine 1-oxides only
4-monosubstitution	1,230–1,210	8·13– 8·26	v.	pyridines only
	1,175–1,165	8·51– 8·59	s.	pyridine 1-oxides only
	1,110–1,095	9·01– 9·13	w.	pyridine 1-oxides only
	1,070–1,065	9·35– 9·39	w.	pyridines only
	1,040–1,030	9·62– 9·71	m.	pyridine 1-oxides only
	850– 790	11·76–12·66	s.	pyridines and 1-oxides
2:3-disubstitution	815– 785	12·27–12·74		o.o.p. vib.
	740– 690	13·51–14·49	m.-s.	
2:5-disubstitution	825– 810	12·12–12·35		o.o.p. vib.
	735– 725	13·60–13·75		
2:6-disubstitution	815– 770	12·27–12·99		o.o.p. vib.
	750– 720	13·33–13·89		
3:4-disubstitution	890– 860	11·24–11·63	s.	pyridine 1-oxides only
	825– 810	12·12–12·35	s.	pyridine-1-oxides only
	860– 840	11·63–11·90	m.	pyridines only

Diazines and Triazines

Stretching Vibrations

=C—H str.	3,090–3,040	3·24–3·29	m.	
Pyrimidines	1,590–1,555	6·29–6·43	v.	
	1,565–1,520	6·39–6·58	v.	
	1,480–1,400	6·76–7·15	v.	
	1,410–1,375	7·09–7·28	v.	
	1,020– 990	9·80–10·10	m.	ring breathing vib.
Pyrazines and pyrazine 1-oxides	1,600–1,575	6·25–6·35	v.	
	1,550–1,520	6·45–6·58	w.-m.	
	1,500–1,465	6·67–6·83	m.-s.	
	1,420–1,370	7·04–7·30	m.-s.	
sym-Triazines	1,560–1,520	6·41–6·58	v.	
	1,490–1,450	6·71–6·90	v.	

Table 13—continued

Pyrylium Salts

Stretching Vibrations

=C—H str.	3,100–3,010	3·20– 3·32	w.-m.	multiple bands
C=C i.p. vib.	1,650–1,615	6·06– 6·19	vs.	
	1,560–1,520	6·41– 6·58	vs.	
	1,520–1,465	6·58– 6·83	m.	
	1,450–1,400	6·90– 7·14	v.	
	1,000– 970	10·00–10·31	v.	ring breathing vib.

C—H *Out-of-plane Deformations*

unsubstituted	*ca.* 960	*ca.* 10·42	s.	
	ca. 775	*ca.* 12·90	m.	o.o.p. ring vib.
2:6-disubstitution	*ca.* 935	*ca.* 10·70	m.	
	ca. 800	*ca.* 12·50	s.	
2:4:6-trisubstitution	960–900	10·42–11·11	v.	two bands. l.v.
	890–870	11·24–11·49	m.	
2:3:4:6-tetra-substitution	925–915	10·81–10·93	w.	l.v.
	900–880	11·11–11·36	w.	l.v.
2:3:5:6-tetra-substitution	710–700	14·08–14·29	m.	

Pyridones, Pyrones, and Related Compounds

Stretching Vibrations

Pyrid-2-ones and -thiones	1,670–1,655	5·99–6·04	vs.	C=O str.
	1,630–1,590	6·14–6·29	vs.	
	1,570–1,535	6·37–6·52	s.	
	1,500–1,470	6·67–6·80	m.	
	1,445–1,415	6·92–7·06	m.-s.	
	1,145–1,100	8·73–9·09	m.-s.	C=S str.
Pyrid-4-ones and -thiones	1,660–1,620	6·02–6·17	vs.	
	1,580–1,550	6·33–6·45	vs.	C=O str.
	1,515–1,485	6·60–6·74	w.-m.	
	1,470–1,400	6·80–7·14	m.-s.	
	1,120–1,105	8·93–9·05	vs.	C=S str.
Pyr-2-ones	1,735–1,730	5·76–5·78	s.	C=O str.
	1,650–1,635	6·06–6·12	m.	
	1,570–1,560	6·37–6·41	s.	
Pyr-4-ones and -thiones*	1,680–1,600	5·95–6·25	vs.	
	1,635–1,525	6·12–6·56	vs.	
	1,465–1,445	6·83–6·92	m.-s.	
	1,420–1,400	7·04–7·14	m.	
	ca. 1,100	*ca.* 9·09	s.	C=S str.

* There is strong coupling of the C = O and C = C stretching vibrations such that no one band may be assigned to the C = O vibration. Thiapyrones and thiapyrthiones absorb at *ca.* 40 cm^{-1} lower frequency.

Table 14. Aromatic Heterocyclic Compounds: Five-membered Rings

Pyrroles

Stretching Vibrations

N—H str. (free bonded)	3,500–3,400	2·86–2·94	v.	
	3,400–3,000	2·94–3·23	s.	broad band
=C—H str.	3,100–3,000	3·23–3·33	m.	
C=C i.p. vib.	1,580–1,545	6·33–6·47	w.	two bands for 1-subst. pyrroles
	1,535–1,525	6·52–6·56	w.	1:2-, 1:2:5-, and 1:3:4-subst. pyrroles only
	1,500–1,475	6·66–6·78	m.-s.	1:2- subst. pyrroles only
	1,480–1,460	6·76–6·85	w.-m.	
	1,430–1,390	6·99–7·19	vs.	

N—H *and* C—H *In- and Out-of-plane deformations*

1-substitution	1,075–1,065	9·30– 9·39	s.	4 adj. H atoms
	1,035–1,015	9·66– 9·85	m.	4 adj. H atoms, l.v.
	930– 920	10·75–10·87	m.	4 adj. H atoms, l.v.
	725– 720	13·79–13·89	vs.	4 adj. H atoms
2-substitution	1,120–1,110	8·93– 9·01	w.-m.	N—H i.p. def.
	1,105–1,070	9·05– 9·35	m.-s.	3 adj. H atoms + NH. l.v.
	1,040–1,020	9·62– 9·80	m.-s.	3 adj. H atoms + NH. l.v.
	930– 925	10·75–10·81	w.	3 adj. H atoms + NH. l.v.
	885– 875	11·30–11·43	w.-m.	3 adj. H atoms + NH
1:2-disubstitution	1,095–1,085	9·13– 9·22	m.	3 adj. H atoms
	1,065–1,050	9·43– 9·52	v.	3 adj. H atoms
1:2:5-trisubstitution	1,040–1,030	9·62– 9·71	m.	2 adj. H atoms. l.v.
	980– 965	10·20–10·36	w.	2 adj. H atoms. l.v.
	760– 750	13·16–13·33	vs.	2 adj. H atoms
1:3:4-trisubstitution	1,060–1,050	9·43– 9·52	s.	isolated H atom
	935– 930	10·70–10·75	m.	isolated H atom
	780– 760	12·82–13·16	vs.	isolated H atom

Thiophens

Stretching Vibrations

=C—H	3,100–3,000	3·23– 3·33	m.	
C=C i.p. str.	1,555–1,480	6·43 –6·76	v.	
	1,445–1,390	6·92– 7·19	v.	
	1,375–1,340	7·28 –7·46	v.	
	1,240–1,195	8·06– 8·37	v.	
	840– 790	11·90–12·66	m.	ring breathing vib. 2-subst. cpds.
	895– 850	11·17–11·76	m.	ring breathing vib. 3-subst. cpds.

Table 14—continued

C—H *In- and Out-of-plane Deformations*

2-substitution	1,085–1,075	9·22– 9·30	w.	l.v.
	1,055–1,030	9·48– 9·71	w.-m.	
	940– 905	10·64–11·05	w.	
	865– 840	11·56–11·90	m.-s.	
3-substitution	1,100–1,070	9·09– 9·35	w.	l.v.
	ca. 1,155	*ca.* 8·66	w.	l.v.
	795– 745	12·58–13·42	s.	

Furans

Stretching Vibrations

=C—H str.	3,100–3,000	3·23– 3·33	m.	
C=C i.p. vib.	1,610–1,560	6·21– 6·41	v.	
	1,515–1,470	6·60– 6·80	v.	
	1,405–1,380	7·11– 7·25	v.	
	1,025–1,005	9·76– 9·95	m.-s.	ring breathing vib.

C—H *In- and Out-of-plane Deformations*

2-substitution	1,240–1,200	8·07– 8·33	v.	
	1,175–1,145	8·51– 8·73	m.-s.	
	1,085–1,070	9·22– 9·35	m.	
	945– 910	10·58–10·99	m.	
	890– 880	11·24–11·36	v.	
	840– 800	11·90–12·50	w.	l.v.
3-substitution	1,170–1,150	8·55– 8·70	s.	
	1,080–1,050	9·26– 9·52	m.-s.	
	1,025–1,005	9·76– 9·95	s.-vs.	
	ca. 920	*ca.* 10·87	v.	l.v.
	880– 870	11·36–11·49	s.	
	790– 720	12·66–13·89	s.	usually two bands

Azoles

The majority of azoles have four absorption bands in the ranges 1,670–1,520 (5·99–6·58), 1,555–1,470 (6·43–6·80), 1,490–1,390 (6·71–7·20), and 1,450–1,320 cm^{-1} (6·90–7·58 μ). Both the positions and the intensities of these bands vary considerably with the orientation of the ring heteroatoms and with the positions and type of the substituents. Although the out-of-plane CH deformation bands for these compounds may be correlated with the number and orientation of the aromatic hydrogen atoms they are of limited value.

Polycyclic Heteroaromatic Compounds

In general, the polycyclic compounds have between four and ten medium to strong bands in the 1,650–1,350 cm^{-1} (6·06–7·41 μ) region, which may be assigned to the aromatic in-plane ring deformations. It appears possible that the overall aromatic substitution pattern may be determined from the

CH deformation frequencies one would expect for the individual rings, e.g., 4-substituted quinolines absorb near 953 and 870 cm^{-1} (10·49–11·49 μ), characteristic of 4 adjacent hydrogen atoms, and near 850 cm^{-1} (11·76 μ), characteristic of 2 adjacent hydrogen atoms (cf. *Tables 12* and *13*).

ALCOHOLS, PHENOLS, ETHERS AND PEROXIDES

Table 15. Alcohols and phenols

O—H *Stretching Vibrations*					
free OH	3,670–3,580	2·73–2·79	v.	sharp band	
hydrogen bonded OH					
(a) intermolecular					
dimeric association	3,550–3,450	2·82–2·90	v.	sharp band	int. changes and frequency shifts on dilution
polymeric association	3,400–3,230	2·94–3·10	s.	broad band	
(b) intramolecular	3,590–3,420	2·79–2·92	v.	sharp band	unaffected by dilution
(c) chelate compounds	3,200–1,700	3·13–5·88	w.	very broad band	
(d) tropolones	*ca.* 3,100	*ca.* 3·23			
—OD	2,780–2,400	3·60–4·17	v.	O—D str.	
C—O *Stretching and* O—H *In-plane Deformations*					
primary alcohol	1,075–1,000	9·30–10·00	s.	l.v.	
	1,350–1,260	7·40– 7·94	s.	l.v.	
secondary alcohol	1,350–1,260	7·40– 7·94	s.	l.v.	
alkyl—CHOH	1,125–1,090	8·89– 9·17	s.	l.v.	
aryl—CHOH	1,075–1,000	9·30–10·00	s.	l.v.	
tertiary alcohol	1,410–1,310	7·09– 7·63	s.	l.v.	
	1,210–1,100	8·26– 9·09	s.	l.v.	
phenols	1,410–1,310	7·09– 7·63	s.	l.v.	
	1,260–1,180	7·94– 8·48	s.	l.v.	

Table 16. Ethers and Peroxides

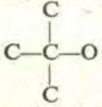
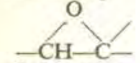
C—O *Stretching Vibrations*				
acyclic CH_2—O—CH_2	1,150–1,060	8·70– 9·43	s.	
 $C-\underset{C}{\overset{C}{C}}-O$	920– 800	10·87–12·50	s.	
aryl and aralkyl ethers	1,310–1,230	7·63– 8·13	s.	X-sensitive band
vinyl ethers	1,225–1,200	8·16– 8·33	s.	
epoxides	1,280–1,240	7·81– 8·07	s.	i.b.
epoxides (*trans*)	950– 860	10·53–11·63	v.	l.v.
epoxides (*cis*)	865– 785	11·56–12·74	m.	l.v.
trimethylene oxides	980– 970	10·20–10·31	s.	
higher cyclic ethers	1,140–1,070	8·77– 9·35	s.	l.v.
—O—CH_2—O—	*ca.* 940	*ca.* 10·65	s.	l.v.
phthalans	915– 895	10·93–11·17	m.	
acetals	1,180–1,040	8·48– 9·62	s.	several bands l.v.

Table 16—continued

C—H *Stretching Vibrations*

$—O—CH_3$	2,895–2,840	3·45– 3·52	m.	
	3,050–2,990	3·28– 3·34	w.	
alkyl acetals, $—CH_2OCHROCH_2—$	*ca.* 2,825	*ca.* 3·54	m.	
$—O—CH_2—O—$	*ca.* 2,780	*ca.* 3·60		
vinyl ethers	3,150–3,050	3·18– 3·28	w.	

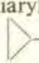
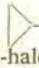
Peroxides, Hydroperoxides, and Peroxy Acids

all peroxy compounds	890– 830	11·24–12·05	w.	O—O str., l.v.
alkyl peroxides	1,150–1,030	8·70– 9·71	m.-s.	C—O str., l.v.
aryl peroxides	*ca.* 1,000	*ca.* 10·00	m.	X-sensitive band, l.v.
R.OOH	*ca.* 3,450	*ca.* 2·90	m.	O—H str.
acyl peroxides	1,820–1,810	5·50– 5·53	s.	C=O str.
	1,800–1,780	5·56– 5·62	s.	
aroyl peroxides	1,805–1,780	5·54– 5·62	s.	
	1,785–1,755	5·60– 5·70	s.	
peroxy acids	*ca.* 3,280	*ca.* 3·05	m.-s.	O—H str.
	ca. 1,760	*ca.* 5·68	s.	C=O str.
	ca. 1,175	*ca.* 8·51	m.-s.	C—O str.
	ca. 865	*ca.* 11·56	w.	O—O str.

KETONES AND ALDEHYDES

*Table 17. Ketones**†*

C=O *Stretching Vibrations*

acyclic	1,725–1,700	5·80– 5·88	s.	
α:β unsat. acyclic compounds	1,700–1,685	5·88– 5·94	s.	s-cis, C=C vib. 1,625–1,615 cm^{-1}
	1,690–1,675	5·92– 5·97	s.	s-trans, C=C vib. 1,645–1,620 cm^{-1}
cross-conj. dienones	1,670–1,660	5·99– 6·02	s.	
aryl ketones	1,700–1,680	5·88– 5·95	s.	
diaryl ketones	1,670–1,660	5·99– 6·02	s.	
—CO.CH_3	1,705–1,680	5·86– 5·95	s.	
—CO.aryl	1,695–1,670	5·90– 5·99	s.	
α-halogenated ketones†				
—CO—CO—	1,730–1,710	5·78– 5·85	s.	
$—CO—CH_2—CO—$				
(keto form)	*ca.* 1,700	*ca.* 5.88	v.	
(enol form)	1,640–1,535	6·10– 6·52	s.	chelated, broad peak
ortho $CO.C_6H_4.OH$ (or NH_2)	1,655–1,610	6·04– 6·21	s.	H bonded
$CO.CH_2CH_2.CO$	1,725–1,705	5·80– 5·87	s.	
$CO.O.CH_2.CO$	1,745–1,725	5·73– 5·80	s.	

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* For influence of physical state and medium on frequency of carbonyl bands see Part I, p. 34.

† For ketones, except those in which hydrogen bonding occurs, additive shifts of the original C=O stretching frequencies, and hence of the range limits given in the table, are observed for α substituents, as opposite

Table 17—continued

Other Vibrations

CH_3—CO—	1,360–1,355	7·35–7·38	s.	CH_3 def.
—CH_2—CO—	1,435–1,405	6·97–7·12	s.	CH_2 def.
alkyl ketones	1,325–1,215	7·55–8·23	m.	l.v.
aryl ketones	1,225–1,075	8·17–9·30	m.	l.v.
C=O	3,550–3,200	2·82–3·13	w.	C=O str. overtones

α substituent	Frequency shift cm^{-1}	Wavelength shift μ	
α:β unsaturation	−30	+0·11	
α halogen	+20	−0·07	in cyclic ketones only equatorial halogen causes +20 cm^{-1} shift
αα′ halogens	+40	−0·15	
αα halogens	+20	−0·07	

Table 18. Cyclic Ketones

C=O *Stretching Vibrations*

9–7 membered rings	*ca.* 1,705	*ca.* 5·87	s.	
6 membered rings	*ca.* 1,720	*ca.* 5·81	s.	
5 membered rings	*ca.* 1,750	*ca.* 5·71	s.	
4 membered rings	*ca.* 1,790	*ca.* 5·59	s.	
ketenes ('2 membered ring')	2,150–2,120	4·56– 4·71	s.	
cyclopropenones	1,645–1,620	6·08– 6·17	s.	
	1,865–1,845	5·36– 5·42	s.	C=C str.
quinones—2 CO's in the same ring	1,690–1,655	5·92– 6·04	s.	
2 CO's in 2 rings	1,655–1,635	6·04– 6·12	s.	
tropones	1,600–1,575	6·25– 6·35	s.	
tropolones	1,620–1,600	6·17– 6·25	s.	H bonded

Table 19. Aldehydes

C=O *Stretching Vibrations*

sat. aliphatic aldehydes	1,740–1,720	5·75–5·81	s.	
α:β-unsat. aldehydes	1,705–1,685	5·78–5·93	s.	
conj. polyene aldehydes	1,680–1,660	5·95–6·02	s.	
aryl aldehydes	1,715–1,695	5·83–5·90	s.	
—C(OH)=C—CHO	1,670–1,645	5·99–6·08	s.	intramolecular H bonding

C—H *Stretching and Deformation Vibrations*

CHO	2,880–2,650	3·47– 3·77	w.-m.	C—H str. 2 bands may appear
	975– 780	10·26–12·82	w.	l.v.; C—H def.

Other Vibrations

aliphatic aldehydes	1,440–1,325	6·94–7·55	m.	l.v.
aryl aldehydes	1,415–1,350	7·07–7·41	m.	l.v.
	1,320–1,260	7·58–7·94	m.	l.v.
	1,230–1,160	8·13–8·62	m.	l.v.

CARBOXYLIC ACIDS AND DERIVATIVES

Table 20. Carboxylic Acids

O—H *Vibrations*				
free OH	3,550–3,500	2·82– 2·86	m.	O—H str.
bonded OH	3,300–2,500	3·00– 4·00	w.	broad band, O—H str.
all OH	955– 890	10·47–11·24	v.	o.o.p. def.
C=O *Stretching Vibrations*				
sat. aliphatic acids	1,725–1,700	5·80–5·88	s.	all acids examined as dimers in so. ph. or liq. ph.
α:β-unsat. acids	1,715–1,680	5·83–5·95	s.	
aryl acids	1,700–1,680	5·88–5·95	s.	
intramolecular H bonded acids	1,680–1,650	5·95–6·06	s.	
α-halogeno acids	1,740–1,715	5·75–5·83	s.	
Other Vibrations				
solid fatty acids	1,350–1,180	7·40–8·48	w.	CH_2 vib., characteristic band patterns
CO_2H	1,440–1,395	6·94–7·17	w.	combination band of C—O str. and OH i.p. def.
	1,320–1,210	7·58–8·26	s.	
carboxylate ion CO_2	1,610–1,550	6·21–6·45	s.	asym. str.
	1,420–1,300	7·04–7·69	m.	sym. str.

Table 21. Acid Halides and Anhydrides

C—O *Stretching Vibrations*				
anhydrides—cyclic	1,310–1,210	7·63–8·26	s.	
acyclic	1,175–1,045	8·51–9·57	s.	
C=O *Stretching Vibrations*				
'5' ring anhydrides	1,870–1,845	5·35– 5·42	s.	
	1,800–1,775	5·56– 5·63	s.	
conj. '5' ring anhydrides	1,860–1,850	5·38– 5·41	s.	
	1,780–1,760	5·62– 5·68	s.	
acyclic anhydrides	1,825–1,815	5·48– 5·51	s.	
	1,755–1,745	5·70– 5·73	s.	
conj. acyclic anhydrides	1,780–1,770	5·62– 5·65	s.	
	1,725–1,715	5·80– 5·83	s.	
alkyl acid chlorides	1,810–1,795	5·53– 5·57	s.	
aryl acid chlorides	1,785–1,765	5·60– 5·67	s.	

*Table 22. Esters and Lactones**

C=O *Stretching Vibrations*

sat. aliphatic esters	1,750–1,720	5·71– 5·81	s.	
α:β unsat. and aryl esters*	1,730–1,705	5·78– 5·86	s.	
enol acetates	1,760–1,745	5·68– 5·73	s.	
carbonates	*ca.* 1,740	*ca.* 5·75	s.	
α-keto esters and α-diesters	1,755–1,740	5·70– 5·75	s.	
enolic β-keto esters	1,655–1,635	6·04– 6·12	s.	chelation
o-hydroxy (amino) benzoates, etc.	1,690–1,670	5·92– 5·99	s.	chelation
γ-keto esters, non-enolic β-keto esters, and γ- (and higher) diesters	1,750–1,735	5·71– 5·76	s.	
β-lactones	*ca.* 1,825	*ca.* 5·48	s.	
γ-lactones	1,795–1,760	5·57– 5.68	s.	
δ-lactones	1,750–1,735	5·71– 5·76	s.	
α:β-unsat. γ-lactones	1,790–1,775	5·59– 5·63	s.	
	1,765–1,740	5·67– 5·75	s.	
β:γ-unsat. γ-lactones	1,805–1,785	5·54– 5·60	s.	

C—O *Stretching Vibrations* (*several bands*)

formates	1,200–1,160	8·33– 8·62	s.	
acetates	1,260–1,230	7·93– 8·13	s.	
propionates and higher esters	1,280–1,160	7·81– 8·62	s.	
carbonates	1,300–1,150	7·69– 8·70	s.	
esters of α:β unsat. aliphatic acids	1,330–1,160	7·52– 8·62	s.	
esters of aromatic acids	1,300–1,100	7·69– 9·09	s.	
enol acetates	1,220–1,200	8·20– 8·33	s.	

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* For α-substituted esters and lactones, other than those in which hydrogen bonding occurs, the following additive shifts of C=O stretching frequency (or wavelength) for individual compounds and range limits apply approximately:

α-substituent	Frequency shift cm^{-1}	Wavelength shift μ	
α:β double bond	−20	+0·07	
α-halogen	+20	−0·07	
αα-halogens	+20	−0·07	2 bands for soln. spec.

AMINES AND IMINES

Table 23. Amines and Imines

N—H *Stretching Vibrations*

primary amines	3,550–3,330	2·82– 3·00	v.	asym. str.
	3,450–3,250	2·90– 3·08	v.	sym. str.
secondary amines	3,500–3,300	2·86– 3·03	v.	
imines	3,400–3,300	2·94– 3·03	v.	l.v.
associated N—H	3,400–3,100	2·94– 3·23	m.	
free N—D	2,600–2,400	3·85– 4·15	v.	

Table 23—continued

N—H *Deformation Vibrations*

primary amines	1,650–1,580	6·06– 6·33	m.-s.	
secondary amines	*ca.* 1,500	*ca.* 6·67	w.	l.v.

C—N *Stretching Vibrations*

aliphatic amines:				
primary	1,090–1,070	9·17– 9·35	w.-m.	l.v.
secondary	1,190–1,130	8·40– 8·85	w.-m.	l.v.
aromatic amines:				
primary	1,330–1,250	7·52– 8·00	s.	X-sensitive band
secondary	1,340–1,260	7·46– 7·94	s.	
tertiary	1,380–1,330	7·25– 7·52	s.	

Other Vibrations

N-Methyl	2,820–2,760	3·55– 3·62	m.-s.	C—H str.

Table 24. Charged Amine Derivatives
(co-ordination complexes, amine hydrochlorides)

NH_3^+ *Stretching and Deformation Vibrations*

NH_3^+	*ca.* 3,380	*ca.* 2·96	m.	NH_3^+ str. } values for soln.
	ca. 3,280	*ca.* 3·05	m.	NH_3^+ str. } spectra only
	3,350–3,150	2·99–3·18	m.	NH_3^+ str., so. ph. spec., intermolecular H bonding, multiple bands may appear
	1,625–1,560	6·15– 6·41	m.	asym. NH_3^+ def.
	1,550–1,505	6·45– 6·65	m.	sym. NH_3^+ def.
	ca. 800	*ca.* 12·50	w.	NH_3^+ rocking

NH_2^+ *Vibrations*

NH_2^+	3,000–2,700	3·33– 3·70	s.	NH_2^+ str. vib.
	1,620–1,560	6·17–6·41	m.-s.	NH_2^+ def.
	ca. 800	*ca.* 12·50	w.	NH_2^+ rocking, l.v.

NH^+ *Vibrations*

$C{=}NH^+$	2,700–2,330	3·70– 4·29	s.	NH^+ str.
all NH^+	2,200–1,800	4·55–5·56	w.-m.	l.v., NH^+ str.

AMIDES, AMINO ACIDS AND RELATED COMPOUNDS

Table 25. Amides

NH *Stretching Vibrations*

primary amides:				
free NH	3,540–3,480	2·83– 2·88	s.	
	3,420–3,380	2·92– 2·96	s.	
bonded NH	3,360–3,320	2·97– 3·01	m.	
	3,220–3,180	3·11– 3·15	m.	
secondary amides:				
free NH (*cis*)	3,440–3,420	2·91– 2·93	s.	
free NH (*trans*)	3,460–3,440	2·89– 2·91	s.	
bonded NH (*cis*)	3,180–3,140	3·15– 3·19	m.	
bonded NH (*trans*)	3,330–3,270	3·00– 3·06	m.	
primary urethanes	3,450–3,200	2·90– 3·13	m.	
secondary urethanes:				
free NH	3,430–3,390	2·92– 2·95	m.	
bonded NH	*ca.* 3,300	*ca.* 3·03	m.	

NH *Deformation Vibrations*

H bonded secondary amides	*ca.* 700	*ca.* 14·3		o.o.p. def., int. falls on dilution. Amide V band

C=O *Stretching Vibrations* (Amide—I band)

primary amides	*ca.* 1,690	*ca.* 5·92	s.	dil. soln. spec.
	ca. 1,650	*ca.* 6·06	s.	so. ph. spec.
secondary amides	1,700–1,665	5·88– 6·01	s.	dil. soln. spec.
	1,680–1,630	5·95– 6·14	s.	so. ph. spec.
tertiary amides	1,670–1,630	5·99– 6·14	s.	dil. soln. or so. ph. spec.
simple β-lactams	1,760–1,730	5·68– 5·78	s.	dil. soln. spec.
ring-fused β-lactams	1,780–1,770	5·62– 5·65	s.	l.v., dil. soln. spec.
simple γ-lactams	*ca.* 1,700	*ca.* 5·88	s.	l.v.
ring-fused γ-lactams	1,750–1,700	5·71– 5·88	s.	
larger-ring cyclic lactams	*ca.* 1,680	*ca.* 5·95	s.	dil. soln. spec.
ureas,				
—NH—CO—NH—	*ca.* 1,660	*ca.* 6·02	s.	
—CO—NH—CO—	1,790–1,720	5·59– 5·81	s.	
	1,710–1,670	5·85– 5·99	s.	
urethanes	1,740–1,690	5·75– 5·92	s.	

Combination Bands of NH *Deformation and* C—N *Stretching Vibrations*

primary amides	1,650–1,620	6·06– 6·17	s.	so. ph. spec.	Amide II band
	1,620–1,590	6·17– 6·31	s.	dil. soln. spec.	
secondary acyclic amides	1,570–1,515	6·37– 6·60	s.	so. ph. spec.	
	1,550–1,510	6·45– 6·62	s.	dil. soln. spec.	
secondary amides	1,305–1,200	7·67– 8·33	m.	l.v., i.p. combination, Amide III	
urethanes	1,530–1,510	6·54– 6·62	s.	Amide II band	

Table 25—continued

Other Vibrations

primary amides	1,420–1,400	7·04– 7·14	m.	l.v.
secondary amides	770– 620	13·00–16·13	m.	l.v., Amide IV band
	630– 530	15·87–18·87	s.	l.v., Amide VI band
urethanes	1,350–1,250	7·41– 8·00	m.-s.	C—N—C=O vib. l.v.
	1,200–1,050	8·33– 9·52	m.-s.	CO.O vib., several bands l.v.

Table 26. Amino-acids, Amido-acids and Related Ionic Molecules

Amino-acids

amino-acids containing an NH_2 group	3,100–2,600	3·23– 3·85	m.	NH_3^+ str.
	1,665–1,585	6·01– 6·31	w.	NH_3^+ def. Amino-acid I band
	1,550–1,485	6·45–6·73	v.	NH_3^+ def. Amino-acid II band
dicarboxylic α-amino-acids	1,755–1,720	5·70–5·81	s.	C=O str., unionized carboxyl
other dicarboxylic amino-acids	1,730–1,700	5·78–5·88	s.	
dicarboxylic amino-acids	1,230–1,215	8·13–8·23	s.	C—O vib.
all amino acids	1,600–1,560	6·25–6·41	s.	ionized carboxyl, C=O str.
	2,760–2,530	3·62–3·95	w.	i.b., l.v.
	2,140–2,080	4·67–4·81	w.	NH_3^+ str., i.b., l.v.
	1,335–1,300	7·49–7·70	m.	i.b.

Amino-acid Salts $H_2N—(C)_n—CO_2^-M^+$

NH_2	3,400–3,200	2·94–3·13	m.	2 bands, NH_2 str.
CO_2^-	1,600–1,560	6·25–6·41	s.	ionized carboxyl C=O str.

Amino-acid Hydrochlorides $H_3N^+—(C)_n—CO_2H\ Cl^-$

NH_3^+	3,130–3,030	3·20–3·30	m.	NH_3^+ str., i.b.
	1,610–1,590	6·21–6·29	w.	NH_3^+ def.
	1,550–1,485	6·45–6·73	v.	NH_3^+ def.
α-amino-acid hydrochlorides	1,755–1,730	5·70–5.78	s.	C=O str.
other amino-acid hydrochlorides	1,730–1,700	5·78–5·88	s.	C=O str.
all amino-acid hydrochlorides	3,030–2,500	3·30– 4·0	w.	series of nearly continuous bands
	ca. 2,000	*ca.* 5·0	w.	
	1,335–1,300	7·49–7·70	m.	
	1,230–1,215	8·13–8·23	s.	C—O vib.

Amido-acids

NH	3,390–3,260	2·95–3·07	m.	N—H str.
α-amido-acids	1,725–1,695	5·80–5·90	s.	C=O str. (acid)
most amido-acids	2,640–2,360	3·79–4·24	w.	ib., l.v.
	1,945–1,835	5·14–5·45	w.	
α-amido-acids	1,620–1,600	6·14–6·25	s.	Amide I band
other amido-acids	1,650–1,620	6·06–6·14	s.	Amide I band
all amido-acids	1,570–1,500	6·37–6·67	s.	Amido II band
	1,230–1,215	8·13–8·23	s.	C—O vib.

NON-AROMATIC UNSATURATED NITROGEN AND NITROGEN-OXYGEN COMPOUNDS

Table 27. Non-aromatic Unsaturated Nitrogen Compounds

$C=N$ *Stretching Vibrations*

aliphatic azomethenes	1,670–1,665	5·99– 6·01	w.	
aryl azomethenes	1,670–1,650	5·99– 6·06	w.-m.	
α:β unsat. azomethenes	1,660–1,635	6·02– 6·12	m.	
oximes	1,690–1,620	5·92– 6·17	w.-m.	
isoureas	1,670–1,655	5·99– 6·04	m.	
amidines	1,685–1,580	5·93– 6·33	s.	
guanidines	1,670–1,500	5·99– 6·67	v.	
cyclic α:β unsat. $C=N$	1,660–1,560	6·02– 6·41	v.	e.g. pyrrolines

$A=B=N$ *Allenic-type Stretching Vibrations*

$N=C=N$	2,155–2,130	4·64– 4·70	vs.	carbodiimides
$N=C=O$	2,275–2,240	4·40– 4·46	vs.	isocyanates
$[R—C=N=N]^+$	2,310–2,135	4·33– 4·47	s.	diazonium salts
$—N=N=N$	2,160–2,120	4·63– 4·72	s.	azides, asym. str.
	1,300–1,275	7·69– 7·84	w.	azides, l.v., sym. str.

$C\equiv N$ *Stretching Vibrations*

sat. nitriles	2,260–2,240	4·43– 4·46	w.-m.	
acyclic α:β-unsat. nitriles	2,235–2,215	4·47– 4·52	s.	
aryl nitriles	2,240–2,220	4·46– 4·51	m.-s.	
isonitriles	2,145–2,135	4·66– 4·47	s.	l.v.
aryl isonitriles	2,125–2,110	4·71– 4·74	s.	l.v.

$N=N$ *Stretching Vibrations*

alkyl azo compounds	1,570–1,555	6·37– 6·43	v.	
α:β unsat. compounds	*ca.* 1,500	*ca.* 6·67	v.	l.v.
unsymmetric aromatic *trans* azo compounds	*ca.* 1,420	*ca.* 7·04		l.v.
cis compounds	*ca.* 1,510	*ca.* 6·62		l.v.

Table 28. Covalent Compounds Containing Nitrogen–Oxygen Bonds

Oximes $R_2C=NOH$

—NOH	3,650–3,500	2·74– 2·86	v.	free O—H str.
	3,300–3,150	3·03– 3·18	v.	bonded O—H str.
	1,690–1,620	5·92– 6·17	m.-w.	$C=N$ str.
	ca. 930	*ca.* 10.75		N—O str.

Table 28—continued

NO_2 *Vibrations, etc.—Nitro Compounds* ($R·NO_2$)

alkyl nitro compounds	998– 914	10·02–10·94	m.-s.	C—N str. (*trans*) l.v.
primary and secondary nitro	917– 875	10·91–11·43	m.-s.	C—N str. (*gauche*) l.v.
	1,565–1,545	6·39– 6·47	s.	asym. NO_2 str.
	1,385–1,360	7·22– 7·35	s.	sym. NO_2 str.
	1,380	7·25	m.	CH_2 def. in —CH_2—NO_2
	655– 605	15·27–16·53	vs.	NO_2 def.
tertiary nitro	1,545–1,530	6·47– 6·54	s.	asym. NO_2 str.
	1,360–1,340	7·35– 7·46	s.	sym. NO_2 str.
α:β-unsat. nitro	1,530–1,510	6·54– 6·62	s.	asym. NO_2 str.
	1,360–1,335	7·35– 7·49	s.	sym. NO_2 str.
α-halogeno nitro	1,580–1,570	6·33– 6·37	s.	asym. NO_2 str.
	1,355–1,340	7·38– 7·46	s.	sym. NO_2 str.
α:α dihalogenonitro	1,600–1,575	6·25– 6·35	s.	asym. NO_2 str.
	1,340–1,325	7·46– 7·55	s.	sym. NO_2 str.
aromatic nitro	1,550–1,510	6·45– 6·62	s.	asym. NO_2 str.
	1,365–1,335	7·33– 7·49	s.	sym. NO_2 str.
	860– 840	11·63–11·90	s.	C—N vib., l.v.
	ca. 750	*ca.* 13·33	s.	i.b., l.v.

NO_2 *Vibrations—Covalent Nitrates* ($R·O·NO_2$)

NO_2	1,655–1,610	6·04–6·21	s.	asym. NO_2 str.
	1,300–1,255	7·69–7·97	s.	sym. NO_2 str.
	870– 855	11·49–11·70	s.	N—O str.
	760– 745	13·16–13·42	m.	NO_2 o.o.p. def.
	710– 695	14·08–14·39	m.	NO_2 def.

NO_2 *Vibrations—Nitramines* ($R_2N·NO_2$)

sat. nitramines	1,585–1,530	6·31– 6·54	s.	asym. NO_2 str.
alkyl nitroguanidines	1,640–1,605	6·10– 6·23	s.	asym. NO_2 str.
aryl nitroguanidines and nitroureas	1,590–1,575	6·29– 6·35	s.	asym. NO_2 str.
all nitramines	1,300–1,260.	7·69– 7·94	s.	sym. NO_2 str.
	790– 770	12·66–12·99	m.	l.v.

NO *Vibrations—Nitroso Compounds* (R·NO)

Aliphatic monomer	1,620–1,540	6·17– 6·49	s.	
Aromatic monomer	1,515–1,490	6·60– 6·71	s.	
Aliphatic dimer	1,420–1,330	7·04– 7·52	s.	*cis* dimer
	1,345–1,320	7·43– 7·58	s.	
	1,290–1,175	7·75– 8·50	s.	*trans* dimer
Aromatic dimer	*ca.* 1,409	*ca.* 7·10	s.	*cis.* dimer
	1,400–1,390	7·14– 7·19	s.	
	1,300–1,250	7·69– 8·00	s.	*trans* dimer

NO *Vibrations—Nitrites* (R—O—N=O)

R—O—N=O *trans* form	1,680–1,650	5·95– 6·06	vs.	N=O str.
cis form	1,625–1,610	6·16– 6·21	vs.	N=O str.
R—O—N=O *trans* form	815– 750	12·27–13·33	s.	N—O str., l.v.
cis form	850– 810	11·76–12·35	s.	N—O str., l.v.
R—O—N=O *cis* form	690– 615	14·49–16·26	s.	O—N=O def., l.v.
trans form	625– 565	16·00–17·70	s.	O—N=O def., l.v.
R—O—N=O	3,360–3,220	2·98– 3·11	m.	N=O str. overtones

Table 28—continued

NO *Vibrations—Nitrosamines* ($R_2N{\cdot}N{=}O$)

N—N=O	1,500–1,480	6·67–6·76	s.	N=O str., vap. ph. spec.
	1,460–1,440	6·85–6·94	s.	N=O str., dil. soln. spec.
	ca. 1,050	*ca.* 9·52	s.	N—N str., l.v.
	ca. 660	*ca.* 15·15	s.	N—N=O def., l.v.

NO *Vibrations—Amine Oxides* (R_3N^+—O^-)

pyridine and pyrimidine N-oxides	1,310–1,220	7·64– 8·20	m.-s.	N—O str., frequency varies widely with ring substituents
	895– 840	11·17–11·90	m.	N—O def.
tert. aliphatic N-oxides	970– 950	10·31–10·53	s.	N—O str., l.v.
aryl nitrile N-oxides	*ca.* 1,370	*ca.* 7·30	s.	N—O str., l.v.

NO *Vibrations—Azoxy Compounds* ($R{\cdot}N{:}N^+$—$O^-{\cdot}R$)

Aromatic compounds	1,480–1,450	6·76– 6·90	m.-s.	asym. N=N—O
	1,335–1,315	7·49– 7·60	m.-s.	sym. N=N—O
Aliphatic compounds	1,530–1,495	6·54– 6·69	m.-s.	

ORGANO-HALOGEN AND ORGANO-SULPHUR COMPOUNDS

Table 29. Organo-Halogen Compounds

Aliphatic C—X *Stretching Vibrations*

C—F monofluorinated compounds	1,110–1,000	9·01–10·00	s.	
C—F difluorinated compounds	1,250–1,050	8·00– 9·50	vs.	2 bands
C—F polyfluorinated compounds	1,400–1,100	7·14– 9·10	vs.	multiple bands
CF_3—CF_2	1,365–1,325	7·33– 7·55	s.	
C—Cl monochlorinated compounds*—primary	730– 650	13·70–15·38	s.	
secondary	675– 610	14·81–16·39	s.	
tertiary	630– 560	15·87–17·86	s.	
C—Cl equatorial	780– 750	12·80–13·33	s.	
C—Cl axial	730– 580	13·70–17·25	s.	
C—Cl polychlorinated compounds	800– 700	12·50–14·30	vs.-s.	l.v.
C—Br*	680– 515	14·71–19·42	s.	
C—Br equatorial	750– 700	13·33–14·29	s.	
C—Br axial	690– 550	14·50–18·20	s.	
C—I	600– 500	16·67–20·00	s.	l.v.

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* Frequency of the band depends upon the geometrical conformation of the molecule. *Trans* isomers absorb at a higher frequency than *gauche* isomers.

Table 29—continued

C—X *Deformation Vibrations*

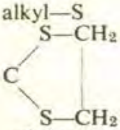
CF_3	1,350–1,120	7·41– 8·93	s.	
	780– 680	12·82–14·71		
CF_2	1,280–1,120	7·81– 8·93	s.	
$CF{-}CF_3$	745– 730	13·42–13·70	s.	
$C{=}CF_2$	1,755–1,735	5·70– 5·76		$C{=}C$ str.
$CF{=}CF_2$	1,800–1,780	5·55– 5·62		$C{=}C$ str.
	1,340–1,300	7·46– 7·69	s.	

Aromatic C—X *Stretching Vibrations* (X-Sensitive Band)

Fluoro compounds	1,270–1,100	7·88– 9·09	m.-s.	
Chloro compounds	1,105–1,035	9·05– 9·66	m.-s.	
Bromo compounds	1,090–1,025	9·18– 9·76	m.-s.	
Iodo compounds	*ca.* 1,060	*ca.* 9·43	m.-s.	

Table 30. Organo–Sulphur Compounds

C—S *Stretching Vibrations*

alkyl—S	705– 570	14·18–17·54	w.	l.v.
	745– 650	13·42–15·38	w.	l.v. several bands
α:β unsat. compounds	*ca.* 740	*ca.* 13·51	v.	
aryl—S	1,110–1,070	9·01– 9·35	m.	X-sensitive band
—CS·S·S·CS—	690– 685	14·49–14·60		l.v.

C=S *Stretching Vibrations*

thioesters	1,225–1,175	8·16– 8·51	s.	
thioureas and thioamides	1,210–1,045	8·26– 9·67	s.	bands resulting from coupling with C—N vib. also found near 1,500 cm^{-1}
$(RS)_2C{=}S$	1,060–1,050	9·43– 9·52	s.	
$(RO)_2\,C{=}S$	1,235–1,210	8·10– 8·26	s.	
$(aryl)_2\,C{=}S$	1,225–1,210	8·17– 8·26	s.	
$-C{=}C{-}C{=}S$	1,155–1,140	8·66– 8·77	s.	
pyrothiones and pyridthiones	1,140–1,110	8·77– 9·01	s.	

S—H *Stretching Vibrations*

	2,590–2,550	3·86–3·92	w.	

Table 30—continued

Other Vibrations

S—CH_3	2,990–2,955	3·34– 3·39	m.-s.	
	2,900–2,865	3·45– 3·49	m.-s.	
	1,440–1,415	6·94– 7·06	m.	
	1,330–1,290	7·52– 7·75	m.-s.	

S=O *Stretching Vibrations*

sat. or unsat. sulphoxides	1,070–1,030	9·35– 9·71	s.	so. ph. spec. 10–20 cm^{-1} lower
$(RO)_2SO$, sulphites	1,220–1,170	8·20– 8·55	s.	
R·SO·OR, sulphinic esters	1,140–1,125	8·77– 8·89	s.	
R·SO·OH, sulphinic acids	1,090– 990	9·17–10·10	s.	
R_2SO_2, sat. or unsat. sulphones	1,350–1,290	7·41– 7·75	vs.	so. ph. spec. 10–20 cm^{-1} lower
	1,165–1,120	8·59– 8·93	vs.	
R·SO_2OH, anhydrous sulphonic acids	1,350–1,340	7·41– 7·46	s.	
	1,165–1,150	8·59– 8·70	s.	S—O str.
	910– 895	10·99–11·17		
hydrated sulphonic acids and RSO_3^-, ionic sulphonates	1,230–1,120	8·13– 8·93	s.	
	1,080–1,025	9·26– 9·76	s.	
R·SO_2OR, covalent sulphonates	1,420–1,330	7·04– 7·52	s.	
	1,200–1,145	8·33– 8·73	s.	
$(RO)_2SO_2$, covalent sulphates	1,440–1,350	6·94– 7·41	s.	
	1,230–1,150	8·13– 8·70	s.	
RSO_2Cl, sulphonyl chlorides	1,390–1,340	7·19– 7·46	s.	
	1,190–1,160	8·40– 8·62	s.	
RSO_2F, sulphonyl fluorides	1,410–1,400	7·09– 7·14	s.	
	1,210–1,200	8·26– 8·33	s.	
RSO_2NR_2, sulphonamides	1,380–1,325	7·25– 7·55	vs.	so. ph. spec. 10–20 cm^{-1} lower
	1,180–1,140	8·48– 8·77	vs.	
	950– 860	10·53–11·63	m.	

PHOSPHORUS, SILICON AND BORON COMPOUNDS

Table 31. Organo-Phosphorus Compounds

P—C *Vibrations, etc.*

P—CH_3	1,430–1,390	6·99– 7·19	m.-s.	asym. CH_3 def.
	1,300–1,275	7·69– 7·85	m.-s.	sym. CH_3 def.
	980– 890	10·20–11·24	s.	CH_3 def.
	790– 770	12·66–12·99	s.	P—C str.
P—CH_2	780– 760	12·82–13·16	s.	P—C str.
P—CH_2 (benzyl)	795– 740	12·58–13·51	s.	P—C str.
P—aryl	1,115–1,090	8·97– 9·17	s.	X-sensitive band
	725– 705	13·79–14·18	s.	X-sensitive band

P—H *Vibrations*

P—H str.	2,450–2,270	4·08– 4·41	m.	
P—D str.	1,795–1,650	5·57– 6·06	m.	

Table 31—continued

P—O *Vibrations, etc.*

P—OH	2,700–2,560	3·70– 3·90	w.	OH str., broad band, strong H bonding
	1,040– 910	9·62–10·99	s.	P—O str.
all P—O-alkyls	1,050– 970	9·52–10.31	vs.	asym. P—O—C str.
P—O— methyl	1,190–1,170	8·40– 8·55	w.	CH_3 def.
P—O— ethyl	1,165–1,155	8·59– 8·68	w.	
P—O— aryl	1,260–1,160	7·94– 8·62	s.	X-sensitive band
	995– 915	10·05–10·93		pentavalent P—O str.
	875– 855	11·43–11·70		trivalent P—O str.
P—O—P	1,000– 870	10·00–11·49	s.	asym. str.
P=O (free)	1,350–1,175	7·41– 8·51	s.	P=O str.
P=O (H bonded)	1,250–1,150	8·00– 8·70	vs.	P=O str.

Table 32. Organo-Silicon Compounds

Si—C *Vibrations*

Si $(CH_3)_n$	1,280–1,255	7·81– 7·97	vs.	sym. CH_3 def.
n = 1	*ca.* 765	*ca.* 13·07	vs.	Si—C str. and CH_3 def.
n = 2	*ca.* 855	*ca.* 11·70	vs.	
	ca. 800	*ca.* 12·50	vs.	
n = 3	*ca.* 840	*ca.* 11·90	vs.	
	ca. 765	*ca.* 13·07	vs.	
Si-phenyl	1,430–1,425	6·99– 7·02	vs.	ring vib.
	1,135–1,090	8·81– 9·17	vs.	X-sensitive band

Si—H *Vibrations*

Si—H str.	2,280–2,080	4·39– 4·81	vs.	
Si—H def.	950– 800	10·53–12·50		

Si—O *Stretching Vibrations*

Si—O—Si and Si—O—C	1,090–1,020	9·17– 9·80	vs.	Si—O str.

Table 33. Boron Compounds

BH	2,565–2,480	3·90– 4·03		BH str.
	1,180–1,110	8·48– 9·01		i.p. def.
	920– 900	10·87–11·11		o.o.p. def.
BH_2	2,640–2,570	3·79– 3·89	s.	sym. str.
	2,530–2,490	3·95– 4·02	s.	asym. str.
	1,170–1,140	8·55– 8·77	m.-s.	i.p. def.
	940– 920	10·64–10·87	m.	o.o.p. def.
B—H · · · · B	1,990–1,850	5·02– 5·40	w.	several bands
	1,610–1,540	6·21– 6·49	s.	
B—CH_3	1,460–1,405	6·85– 7·12	m.	CH_3 sym. def.
	1,320–1,280	7·58– 7·81	m.	CH_3 asym. def.
B—aryl	1,440–1,430	6·94– 6·99	m.-s.	ring. vib.
	1,280–1,220	7·81– 8·20	m.	X-sensitive band
B—O	1,350–1,310	7·41– 7·63	s.	B—O str.
B—N	1,465–1,330	6·83– 7·52	s.	B—N str.
B—Cl (alkylphenyl chloroborinates)	910– 890	10·99–11·24	s.	B—Cl str.

INORGANIC IONS, Etc.

Table 34. Inorganic Ions, Etc.

AsO_4^{3-}	*ca.* 800	*ca.* 12·50	s.	
AsF_6^-	705– 690	14·18–14·49	vs.	
BH_4^-	2,400–2,200	4·17– 4·55	s.	1 or more bands
	1,130–1,040	8·85– 9·62	s.	
BF_4^-	*ca.* 1,060	*ca.* 9·43	vs.	
	ca. 1,030	*ca.* 9·71	vs.	
BrO_3^-	810– 790	12·35–12·66	vs.	
CO_3^{2-}	1,450–1,410	6·90– 7·09	vs.	
	880– 800	11·36–12·50	m.	
HCO_3^-	1,420–1,400	7·04– 7·14	s.	
	1,000– 990	10·00–10·10	s.	
	840– 830	11·90–12·05	s.	
	705– 695	14·18–14·39	s.	
ClO_3^-	980– 930	10·20–10·75	vs.	
ClO_4^-	1,140–1,060	8·77– 9·43	vs.	broad absorption
CrO_4^{2-}	950– 800	10·53–12·50	s.	complex strong bands
$Cr_2O_7^{2-}$	950– 900	10·35–11·11	s.	
CN^-, CNO^-, and CNS^-	2,200–2,000	4·55– 5·00	s.	
CO	2,100–2,000	4·76– 5·00	s.	normal carbonyls
	ca. 1,830	*ca.* 5·46	s.	bridged carbonyls
HF_2^-	*ca.* 1,450	*ca.* 6·90	s.	
	ca. 1,230	*ca.* 8·13	s.	
IO_3^-	800– 700	12·50–14·29	s.	complex strong bands
MnO_4^-	920– 890	10·87–11·24	vs.	
	850– 840	11·76–11·90	m.	
NH_4^+	3,335–3,030	3·00– 3·30	vs.	
	1,485–1,390	6·73– 7·19	s.	
N_3^-	2,170–2,080	4·61– 4·81	s.	
	1,375–1,175	7·27– 8·51	w.	
NO_2^-	1,400–1,300	7·14– 7·69	s.	2 bands in complex nitrites
	1,250–1,230	8·00– 8·13	vs.	
	840– 800	11·90–12·50	w.	
NO_3^-	1,410–1,340	7·09– 7·46	vs.	
	860– 800	11·63–12·50	m.	
NO_2^+	1,410–1,370	7·09– 7·30	s.	
NO^+	2,370–2,230	4·22– 4·48	s.	
NO^+ (coordination comps.)	1,940–1,630	5·16– 6·14	s.	
NO^- (coordination comps.)	1,170–1,045	8·55– 9·57	s.	
NO (nitrosyl halides)	1,850–1,790	5·41– 5·59	s.	
PF_6^-	850– 840	11·76–11·90	vs.	
PO_4^{3-}, HPO_4^{2-}, and $H_2PO_4^-$	1,100– 950	9·09–10·53	s.	
$S_2O_3^{2-}$	1,660–1,620	6·02– 6·17	w.	
	1,000– 990	10·00–10·10	s.	
SO_4^{2-}	1,130–1,080	8·85– 9·26	vs.	
	680– 610	14·71–16·40	m.	
HSO_4^-	1,180–1,160	8·84– 8·62	s.	
	1,080–1,000	9·26–10·00	s.	
	880– 840	11·36–11·90	s.	
SO_3^{2-}	*ca.* 1,100	*ca.* 9·09	v.	l.v.
SeO_4^{2-}	*ca.* 830	*ca.* 12·05	s.	
SiF_6^{2-}	*ca.* 725	*ca.* 13·79	s.	
all silicates	1,100– 900	9·09–11·11	s.	
UO_2^{2+}	940– 900	10·64–11·11	s.	

RECIPROCALS

SUBTRACT

	0	1	2	3	4	5	6	7	8	9	1	2	3	4	5	6	7	8	9
1·0	1·0000	·9901	·9804	·9709	·9615	·9524	·9434	·9346	·9259	·9174	9	18	27	36	45	55	64	73	82
1·1	·9091	·9009	·8929	·8850	·8772	·8696	·8621	·8547	·8475	·8403	8	15	23	30	38	45	53	61	68
1·2	·8333	·8264	·8197	·8130	·8065	·8000	·7937	·7874	·7813	·7752	6	13	19	26	32	38	45	51	58
1·3	·7692	·7634	·7576	·7519	·7463	·7407	·7353	·7299	·7246	·7194	5	11	16	22	27	33	38	44	49
1·4	·7143	·7092	·7042	·6993	·6944	·6897	·6849	·6803	·6757	·6711	5	10	14	19	24	29	33	38	43
1·5	·6667	·6623	·6579	·6536	·6494	·6452	·6410	·6369	·6329	·6289	4	8	13	17	21	25	29	33	38
1·6	·6250	·6211	·6173	·6135	·6098	·6061	·6024	·5988	·5952	·5917	4	7	11	15	18	22	26	29	33
1·7	·5882	·5848	·5814	·5780	·5747	·5714	·5682	·5650	·5618	·5587	3	7	10	13	16	20	23	26	30
1·8	·5556	·5525	·5495	·5464	·5435	·5405	·5376	·5348	·5319	·5291	3	6	9	12	15	18	20	23	26
1·9	·5263	·5236	·5208	·5181	·5155	·5128	·5102	·5076	·5051	·5025	3	5	8	11	13	16	18	21	24
2·0	·5000	·4975	·4950	·4926	·4902	·4878	·4854	·4831	·4808	·4785	2	5	7	10	12	14	17	19	21
2·1	·4762	·4739	·4717	·4695	·4673	·4651	·4630	·4608	·4587	·4566	2	4	7	9	11	13	15	17	20
2·2	·4545	·4525	·4505	·4484	·4464	·4444	·4425	·4405	·4386	·4367	2	4	6	8	10	12	14	16	18
2·3	·4348	·4329	·4310	·4292	·4274	·4255	·4237	·4219	·4202	·4184	2	4	5	7	9	11	13	14	16
2·4	·4167	·4149	·4132	·4115	·4098	·4082	·4065	·4049	·4032	·4016	2	3	5	7	8	10	12	13	15
2·5	·4000	·3984	·3968	·3953	·3937	·3922	·3906	·3891	·3876	·3861	2	3	5	6	8	9	11	12	14
2·6	·3846	·3831	·3817	·3802	·3788	·3774	·3759	·3745	·3731	·3717	1	3	4	6	7	8	10	11	13
2·7	·3704	·3690	·3676	·3663	·3650	·3636	·3623	·3610	·3597	·3584	1	3	4	5	7	8	9	11	12
2·8	·3571	·3559	·3546	·3534	·3521	·3509	·3497	·3484	·3472	·3460	1	2	4	5	6	7	9	10	11
2·9	·3448	·3436	·3425	·3413	·3401	·3390	·3378	·3367	·3356	·3344	1	2	3	5	6	7	8	9	10
3·0	·3333	·3322	·3311	·3300	·3289	·3279	·3268	·3257	·3247	·3236	1	2	3	4	5	6	7	9	10
3·1	·3226	·3215	·3205	·3195	·3185	·3175	·3165	·3155	·3145	·3135	1	2	3	4	5	6	7	8	9
3·2	·3125	·3115	·3106	·3096	·3086	·3077	·3067	·3058	·3049	·3040	1	2	3	4	5	6	7	8	9
3·3	·3030	·3021	·3012	·3003	·2994	·2985	·2976	·2967	·2959	·2950	1	2	3	4	4	5	6	7	8
3·4	·2941	·2933	·2924	·2915	·2907	·2899	·2890	·2882	·2874	·2865	1	2	3	3	4	5	6	7	8
3·5	·2857	·2849	·2841	·2833	·2825	·2817	·2809	·2801	·2793	·2786	1	2	2	3	4	5	6	6	7
3·6	·2778	·2770	·2762	·2755	·2747	·2740	·2732	·2725	·2717	·2710	1	2	2	3	4	5	5	6	7
3·7	·2703	·2695	·2688	·2681	·2674	·2667	·2660	·2653	·2646	·2639	1	1	2	3	4	4	5	6	6
3·8	·2632	·2625	·2618	·2611	·2604	·2597	·2591	·2584	·2577	·2571	1	1	2	3	3	4	5	5	6
3·9	·2564	·2558	·2551	·2545	·2538	·2532	·2525	·2519	·2513	·2506	1	1	2	3	3	4	4	5	6
4·0	·2500	·2494	·2488	·2481	·2475	·2469	·2463	·2457	·2451	·2445	1	1	2	2	3	4	4	5	5
4·1	·2439	·2433	·2427	·2421	·2415	·2410	·2404	·2398	·2392	·2387	1	1	2	2	3	3	4	5	5
4·2	·2381	·2375	·2370	·2364	·2358	·2353	·2347	·2342	·2336	·2331	1	1	2	2	3	3	4	4	5
4·3	·2326	·2320	·2315	·2309	·2304	·2299	·2294	·2288	·2283	·2278	1	1	2	2	3	3	4	4	5
4·4	·2273	·2268	·2262	·2257	·2252	·2247	·2242	·2237	·2232	·2227	1	1	2	2	3	3	4	4	5
4·5	·2222	·2217	·2212	·2208	·2203	·2198	·2193	·2188	·2183	·2179	0	1	1	2	2	3	3	4	4
4·6	·2174	·2169	·2165	·2160	·2155	·2151	·2146	·2141	·2137	·2132	0	1	1	2	2	3	3	4	4
4·7	·2128	·2123	·2119	·2114	·2110	·2105	·2101	·2096	·2092	·2088	0	1	1	2	2	3	3	4	4
4·8	·2083	·2079	·2075	·2070	·2066	·2062	·2058	·2053	·2049	·2045	0	1	1	2	2	3	3	3	4
4·9	·2041	·2037	·2033	·2028	·2024	·2020	·2016	·2012	·2008	·2004	0	1	1	2	2	2	3	3	4
5·0	·2000	·1996	·1992	·1988	·1984	·1980	·1976	·1972	·1969	·1965	0	1	1	2	2	2	3	3	4
5·1	·1961	·1957	·1953	·1949	·1946	·1942	·1938	·1934	·1931	·1927	0	1	1	2	2	2	3	3	3
5·2	·1923	·1919	·1916	·1912	·1908	·1905	·1901	·1898	·1894	·1890	0	1	1	1	2	2	3	3	3
5·3	·1887	·1883	·1880	·1876	·1873	·1869	·1866	·1862	·1859	·1855	0	1	1	1	2	2	3	3	3
5·4	·1852	·1848	·1845	·1842	·1838	·1835	·1832	·1828	·1825	·1821	0	1	1	1	2	2	2	3	3
	0	1	2	3	4	5	6	7	8	9	1	2	3	4	5	6	7	8	9

RECIPROCALS

SUBTRACT

	0	1	2	3	4	5	6	7	8	9	1	2	3	4	5	6	7	8	9
5·5	·1818	·1815	·1812	·1808	·1805	·1802	·1799	·1795	·1792	·1789	0	1	1	1	2	2	2	3	3
5·6	·1786	·1783	·1779	·1776	·1773	·1770	·1767	·1764	·1761	·1757	0	1	1	1	2	2	2	3	3
5·7	·1754	·1751	·1748	·1745	·1742	·1739	·1736	·1733	·1730	·1727	0	1	1	1	2	2	2	2	3
5·8	·1724	·1721	·1718	·1715	·1712	·1709	·1706	·1704	·1701	·1698	0	1	1	1	1	2	2	2	3
5·9	·1695	·1692	·1689	·1686	·1684	·1681	·1678	·1675	·1672	·1669	0	1	1	1	1	2	2	2	3
6·0	·1667	·1664	·1661	·1658	·1656	·1653	·1650	·1647	·1645	·1642	0	1	1	1	1	2	2	2	3
6·1	·1639	·1637	·1634	·1631	·1629	·1626	·1623	·1621	·1618	·1616	0	1	1	1	1	2	2	2	2
6·2	·1613	·1610	·1608	·1605	·1603	·1600	·1597	·1595	·1592	·1590	0	1	1	1	1	2	2	2	2
6·3	·1587	·1585	·1582	·1580	·1577	·1575	·1572	·1570	·1567	·1565	0	0	1	1	1	1	2	2	2
6·4	·1563	·1560	·1558	·1555	·1553	·1550	·1548	·1546	·1543	·1541	0	0	1	1	1	1	2	2	2
6·5	·1538	·1536	·1534	·1531	·1529	·1527	·1524	·1522	·1520	·1517	0	0	1	1	1	1	2	2	2
6·6	·1515	·1513	·1511	·1508	·1506	·1504	·1502	·1499	·1497	·1495	0	0	1	1	1	1	2	2	2
6·7	·1493	·1490	·1488	·1486	·1484	·1481	·1479	·1477	·1475	·1473	0	0	1	1	1	1	2	2	2
6·8	·1471	·1468	·1466	·1464	·1462	·1460	·1458	·1456	·1453	·1451	0	0	1	1	1	1	2	2	2
6·9	·1449	·1447	·1445	·1443	·1441	·1439	·1437	·1435	·1433	·1431	0	0	1	1	1	1	1	2	2
7·0	·1429	·1427	·1425	·1422	·1420	·1418	·1416	·1414	·1412	·1410	0	0	1	1	1	1	1	2	2
7·1	·1408	·1406	·1404	·1403	·1401	·1399	·1397	·1395	·1393	·1391	0	0	1	1	1	1	1	2	2
7·2	·1389	·1387	·1385	·1383	·1381	·1379	·1377	·1376	·1374	·1372	0	0	1	1	1	1	1	2	2
7·3	·1370	·1368	·1366	·1364	·1362	·1361	·1359	·1357	·1355	·1353	0	0	1	1	1	1	1	2	2
7·4	·1351	·1350	·1348	·1346	·1344	·1342	·1340	·1339	·1337	·1335	0	0	1	1	1	1	1	1	2
7·5	·1333	·1332	·1330	·1328	·1326	·1325	·1323	·1321	·1319	·1318	0	0	1	1	1	1	1	1	2
7·6	·1316	·1314	·1312	·1311	·1309	·1307	·1305	·1304	·1302	·1300	0	0	1	1	1	1	1	1	2
7·7	·1299	·1297	·1295	·1294	·1292	·1290	·1289	·1287	·1285	·1284	0	0	0	1	1	1	1	1	1
7·8	·1282	·1280	·1279	·1277	·1276	·1274	·1272	·1271	·1269	·1267	0	0	0	1	1	1	1	1	1
7·9	·1266	·1264	·1263	·1261	·1259	·1258	·1256	·1255	·1253	·1252	0	0	0	1	1	1	1	1	1
8·0	·1250	·1248	·1247	·1245	·1244	·1242	·1241	·1239	·1238	·1236	0	0	0	1	1	1	1	1	1
8·1	·1235	·1233	·1232	·1230	·1229	·1227	·1225	·1224	·1222	·1221	0	0	0	1	1	1	1	1	1
8·2	·1220	·1218	·1217	·1215	·1214	·1212	·1211	·1209	·1208	·1206	0	0	0	1	1	1	1	1	1
8·3	·1205	·1203	·1202	·1200	·1199	·1198	·1196	·1195	·1193	·1192	0	0	0	1	1	1	1	1	1
8·4	·1190	·1189	·1188	·1186	·1185	·1183	·1182	·1181	·1179	·1178	0	0	0	1	1	1	1	1	1
8·5	·1176	·1175	·1174	·1172	·1171	·1170	·1168	·1167	·1166	·1164	0	0	0	1	1	1	1	1	1
8·6	·1163	·1161	·1160	·1159	·1157	·1156	·1155	·1153	·1152	·1151	0	0	0	1	1	1	1	1	1
8·7	·1149	·1148	·1147	·1145	·1144	·1143	·1142	·1140	·1139	·1138	0	0	0	1	1	1	1	1	1
8·8	·1136	·1135	·1134	·1133	·1131	·1130	·1129	·1127	·1126	·1125	0	0	0	1	1	1	1	1	1
8·9	·1124	·1122	·1121	·1120	·1119	·1117	·1116	·1115	·1114	·1112	0	0	0	1	1	1	1	1	1
9·0	·1111	·1110	·1109	·1107	·1106	·1105	·1104	·1103	·1101	·1100	0	0	0	1	1	1	1	1	1
9·1	·1099	·1098	·1096	·1095	·1094	·1093	·1092	·1091	·1089	·1088	0	0	0	0	1	1	1	1	1
9·2	·1087	·1086	·1085	·1083	·1082	·1081	·1080	·1079	·1078	·1076	0	0	0	0	1	1	1	1	1
9·3	·1075	·1074	·1073	·1072	·1071	·1070	·1068	·1067	·1066	·1065	0	0	0	0	1	1	1	1	1
9·4	·1064	·1063	·1062	·1060	·1059	·1058	·1057	·1056	·1055	·1054	0	0	0	0	1	1	1	1	1
9·5	·1053	·1052	·1050	·1049	·1048	·1047	·1046	·1045	·1044	·1043	0	0	0	0	1	1	1	1	1
9·6	·1042	·1041	·1040	·1038	·1037	·1036	·1035	·1034	·1033	·1032	0	0	0	0	1	1	1	1	1
9·7	·1031	·1030	·1029	·1028	·1027	·1026	·1025	·1024	·1022	·1021	0	0	0	0	1	1	1	1	1
9·8	·1020	·1019	·1018	·1017	·1016	·1015	·1014	·1013	·1012	·1011	0	0	0	0	1	1	1	1	1
9·9	·1010	·1009	·1008	·1007	·1006	·1005	·1004	·1003	·1002	·1001	0	0	0	0	0	1	1	1	1
	0	1	2	3	4	5	6	7	8	9	1	2	3	4	5	6	7	8	9

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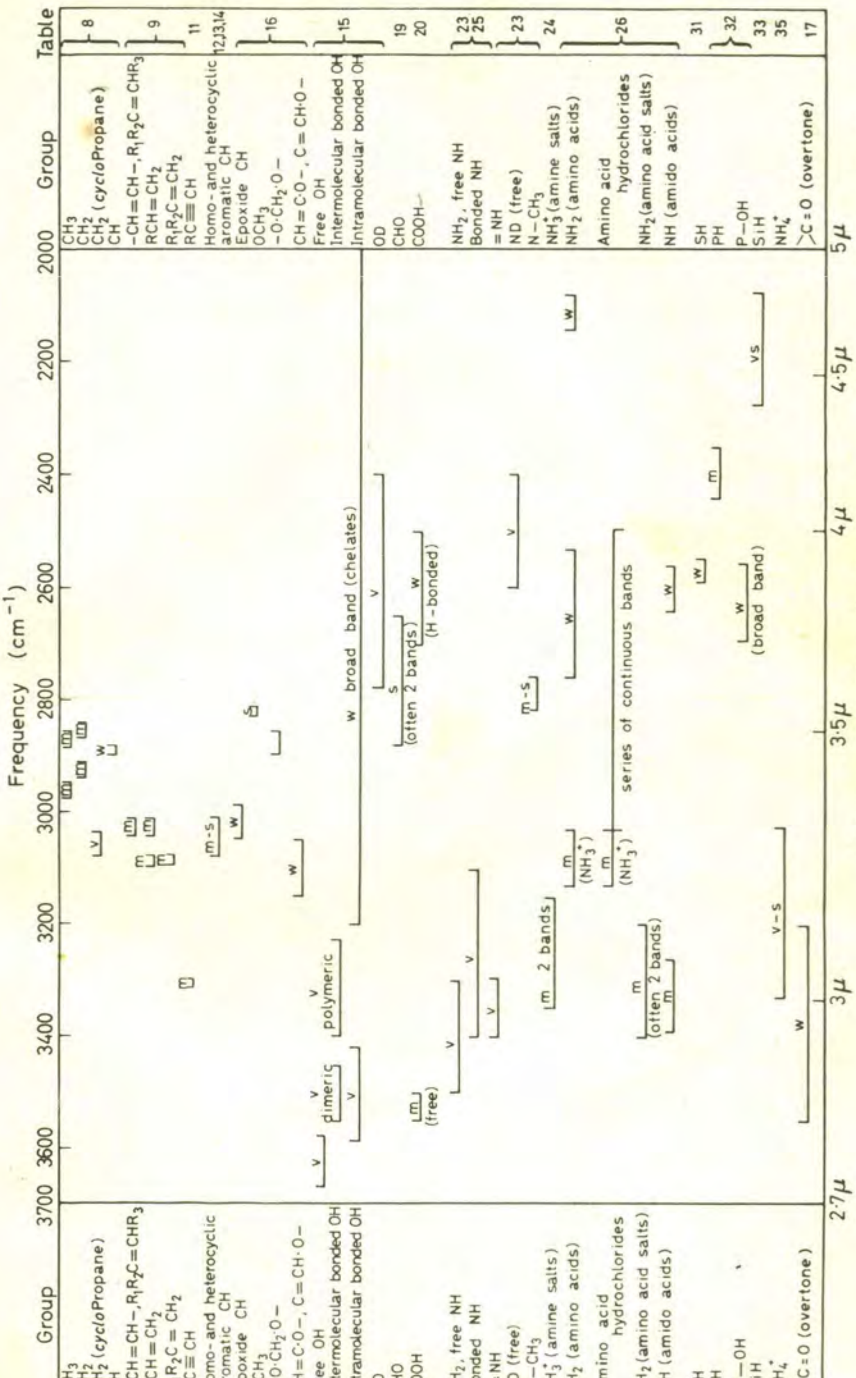
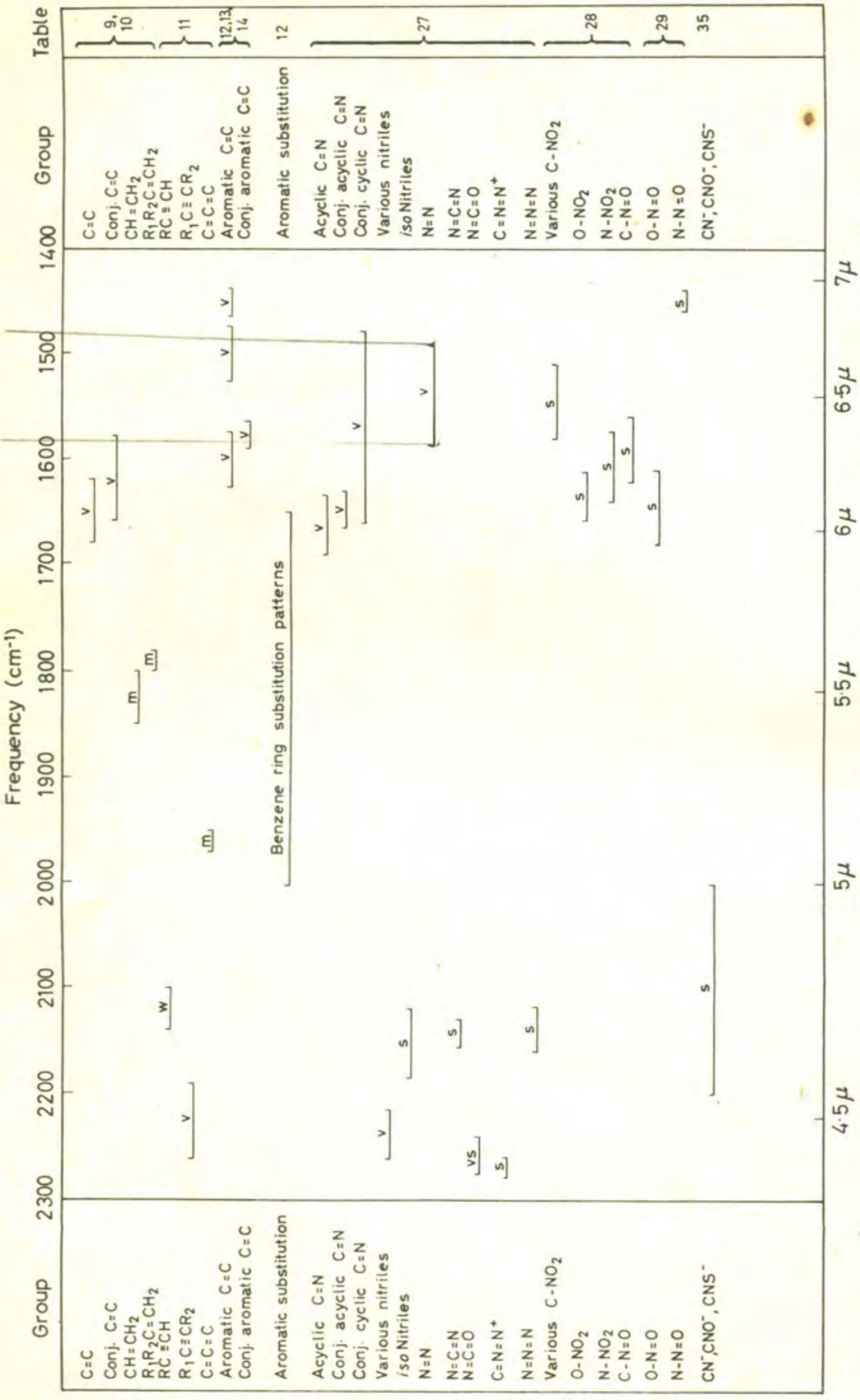
ABBREVIATIONS

adj.	adjacent	s.	strong intensity
approx.	approximately	sat.	saturated
asym.	asymmetrical	sec.	secondary
conj.	conjugated	soln.	solution
def.	deformation	so. ph.	solid phase
dil.	dilute	spec.	spectrum
enh.	enhanced	str.	stretching
i.b.	inconsistent band	sym.	symmetrical
int.	intensity	tert.	tertiary
i.p.	in-plane	unsat.	unsaturated
liq. ph.	liquid phase	v.	variable intensity
l.v.	limited value assignment	vap. ph.	vapour phase
m.	medium intensity	vib.	vibration
non-conj.	non-conjugated	v.s.	very strong intensity
o.o.p.	out-of-plane	w.	weak intensity
'5' ring	5-membered ring, etc.		



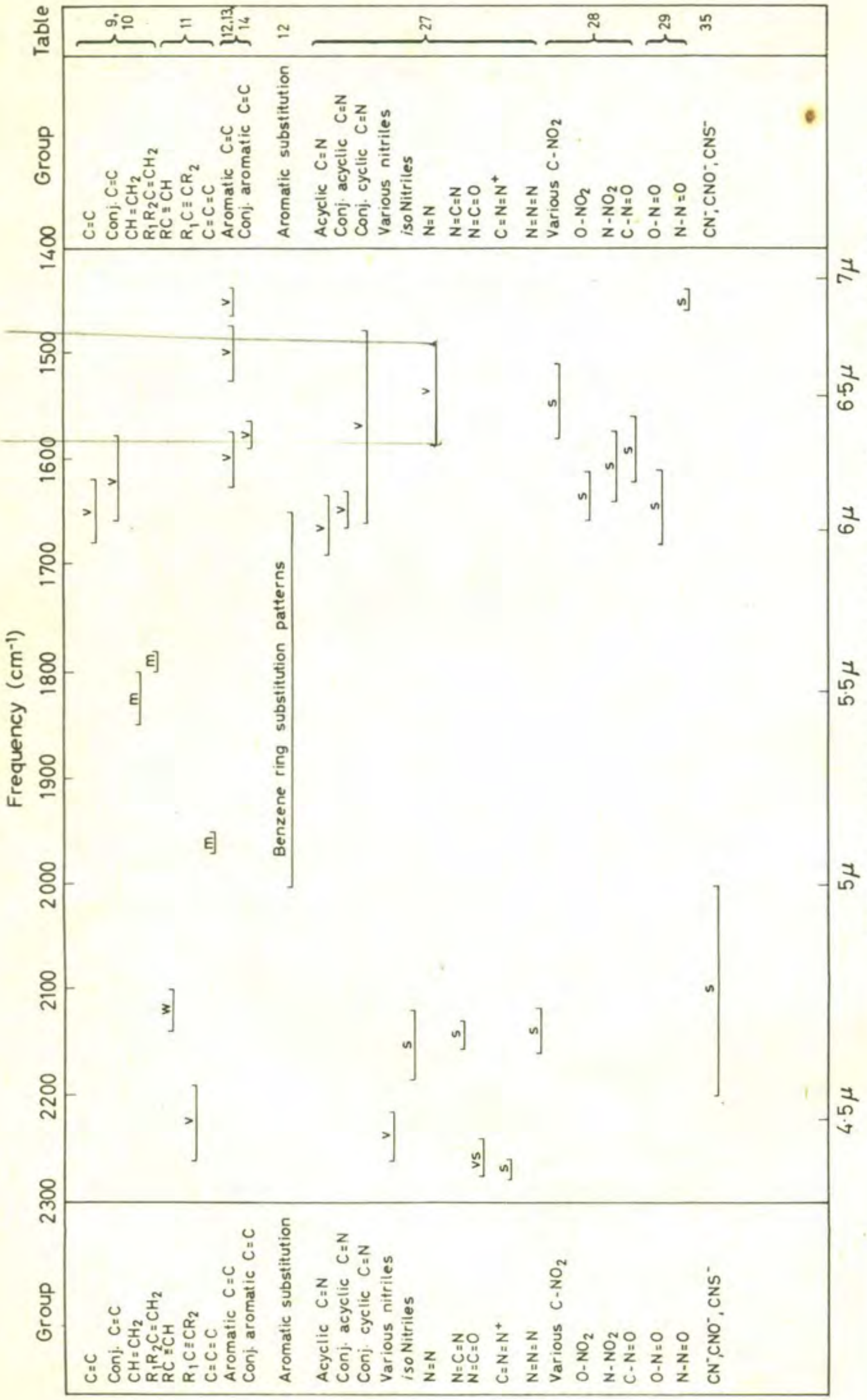
Hydrogen stretching vibrations etc.

Correlation Chart I



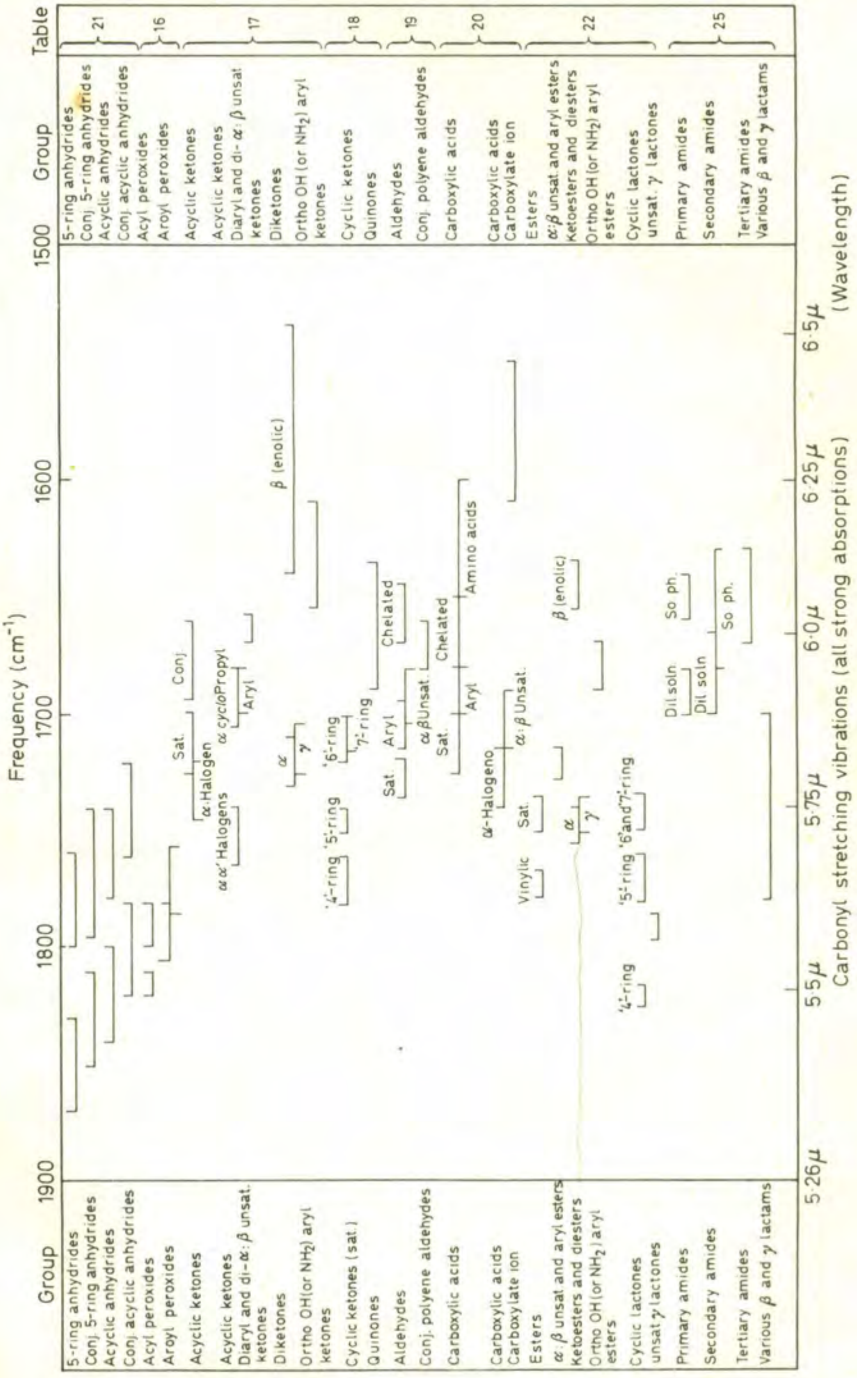
Multiple bond vibrations etc. (excluding C=O)

Correlation Chart II

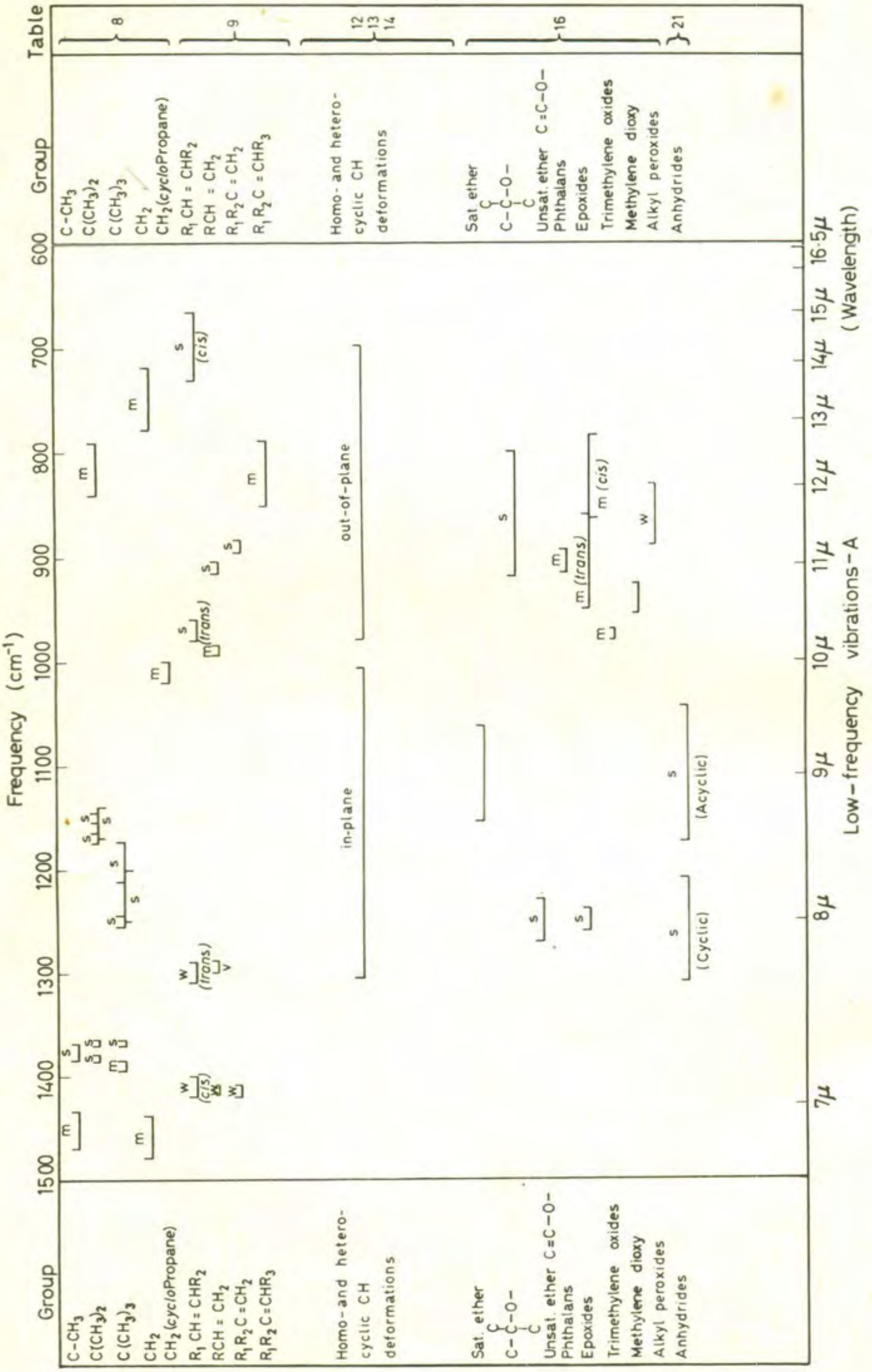


Multiple bond vibrations etc. (excluding C=O)

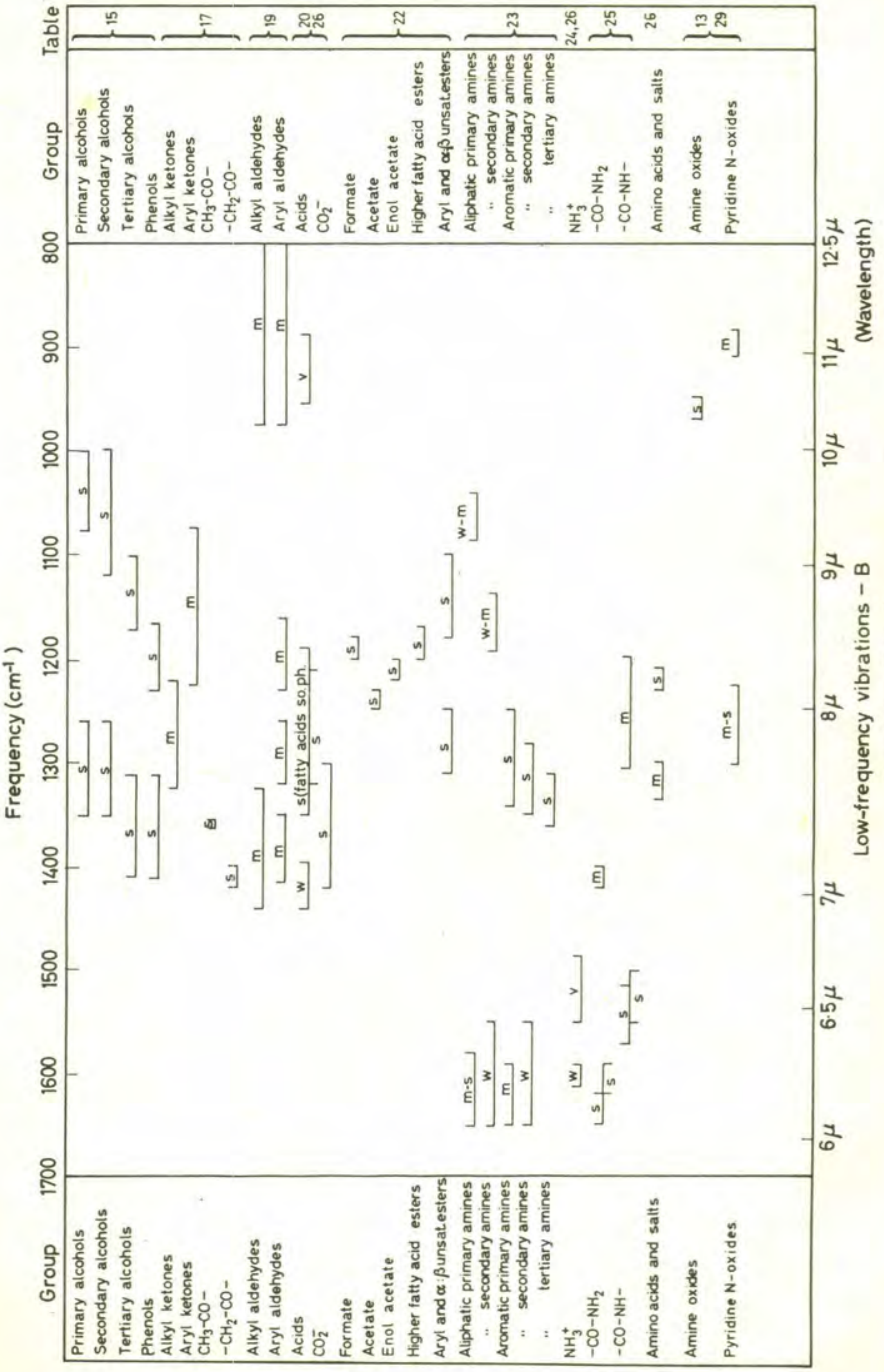
Correlation Chart II



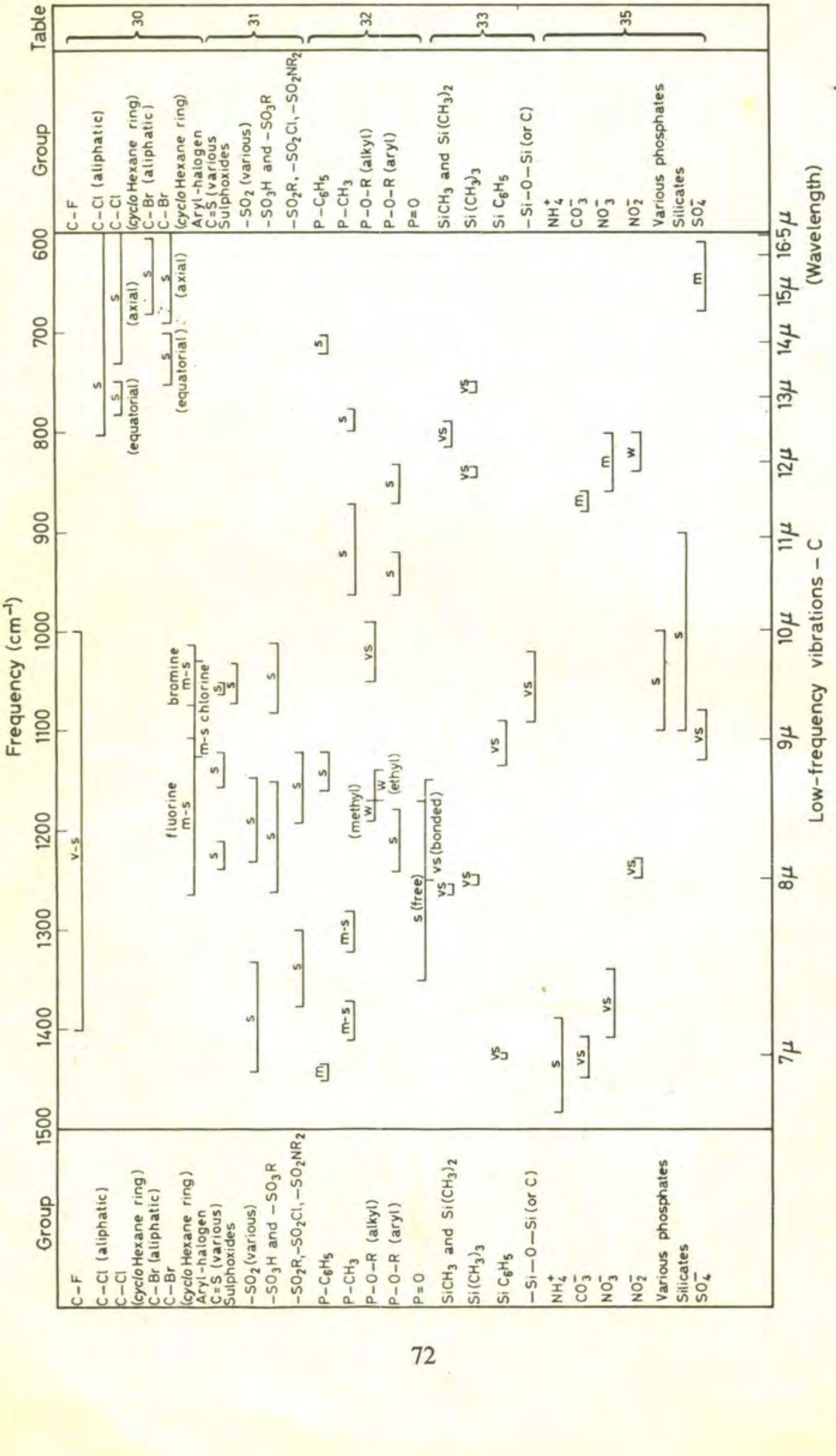
Correlation Chart III



Correlation Chart IV



Correlation Chart V



Low-frequency vibrations – C

Correlation Chart VI

For boron compounds and many inorganic ions the tables should be consulted.

ALKANES

Table 8. Alkanes and Cycloalkanes*

C—H *Stretching Vibrations*

Alkyl—CH_3	2,975–2,950	3·36–3·39	m.	The presence of several of these groups gives strong absorption.
	2,885–2,860	3·47–3·50	m.	
Aryl—CH_3	2,930–2,920	3·41–3·43	m.	
	2,870–2,860	3·48–3·50	m.	
acyclic—CH_2—	2,940–2,915	3·40–3·45	m.	
	2,870–2,845	3·49–3·52	m.	
acyclic—CH—	2,900–2,880	3·45–3·47	w.	
*cyclo*propanes	3,100–3,070	3·23–3·26	v.	
	3,030–2,995	3·30–3·34	v.	
*cyclo*butanes	2,990–2,980	3·34–3·36	v.	
	2,925–2,875	3·42–3·48	v.	
*cyclo*pentanes	2,960–2,950	3·38–3·39	v.	
	2,870–2,850	3·48–3·51	v.	
*cyclo*hexanes	2,940–2,910	3·40–3·44	v.	
	2,870–2,840	3·49–3·52	v.	

C—H *Deformation Vibrations*

C—CH_3	1,470–1,435	6·80–6·97	m.	asym. def.
	1,385–1,370	7·22–7·30	s.	sym. def.
$C(CH_3)_2$	1,385–1,380	7·22–7·25	s.	doublet of approx. equal int.
	1,370–1,365	7·30–7·33	s.	
$C(CH_3)_3$	1,400–1,390	7·14–7·19	m.	doublet int. ratio *ca.* 1:2
	1,375–1,365	7·27–7·33	s.	
—CH_2—	1,480–1,440	6·76–6·94	m.	CH_2 scissor
—CH—	*ca.* 1,340	*ca.* 7·46	w.	l.v.

Skeletal Vibrations

$C(CH_3)_2$	1,175–1,165	8·51– 8·58	s.	
	1,150–1,130	8·90– 8·85	s.	
	840– 790	11·90–12·66	m.	l.v.
$C(CH_3)_3$	1,255–1,245	7·97– 8·03	s.	
	1,210–1,160	8·26– 8·62	s.	
acyclic—$(CH_2)_n$—				
n = 4 or more	725– 720	13·79–13·89	m.	
n = 3	730– 725	13·70–13·79	m.	
n = 2	740– 735	13·51–13·65	m.	
n = 1	785– 770	12·74–12·99	m.	
*cyclo*propane	1,050–1,000	9·52–10·00	m.	l.v.

---

* For absorption due to OCH_3, NCH_3, etc. see ethers, amines, etc.

ALKENES, ALKYNES, AND ALLENES

Table 9. Alkenes

$C=C$ *Stretching Vibrations*

non-conj. $C=C$	1,680–1,620	5·95–6·17	v.	
$CHR=CH_2$	1,645–1,640	6·08–6·10	v.	
$CHR_1=CHR_2$ (*cis*)	1,665–1,635	6·01–6·12	v.	
$CHR_1=CHR_2$ (*trans*)	1,675–1,665	5·97–6·00	v.	
$CR_1R_2=CH_2$	1,660–1,640	6·02–6·10	v.	
$CR_1R_2=CHR_3$	1,690–1,670	5·92–5·99	v.	
$CR_1R_2=CR_3R_4$	1,690–1,670	5·92–5·99	w.	l.v.
aryl—$C=C$	*ca.* 1,625	*ca.* 6·16	s.	enh. int.
$C=C{\cdot}C=O$ or $C=C{\cdot}C=C$	1,660–1,580	6·02–6·33	s.	cisoid form int. often more enh. than transoid

C—H *Stretching and Deformation Vibrations*

$CHR_1=CH_2$	3,040–3,010	3·29– 3·32	m.	CH str. (CHR_1)
	3,095–3,075	3·23– 3·25	m.	CH str. (CH_2)
	995– 985	10·05–10·15	m.	CH o.o.p. def.
	915– 905	10·93–11·05	s.	CH_2 o.o.p. def.
	1,850–1,800	5·41– 5·56	m.	overtone
	1,420–1,410	7·04– 7·09	w.	CH_2 i.p. def.
	1,300–1,290	7·69– 7·75	v.	CH i.p. def.
$CHR_1=CHR_2$ (*cis*)	3,050–3,000	3·28– 3·33	m.	CH str.
	1,420–1,400	7·04– 7·14	w.	CH i.p. def.
	730– 665	13·70–15·04	s.	CH o.o.p. def.
$CHR_1=CHR_2$ (*trans*)	3,050–3,000	3·28– 3·33	m.	CH str.
	980– 960	10·20–10·42	s.	CH o.o.p. def.
	1,310–1,290	7·63– 7·75	w.	CH i.p. def.
$CR_1R_2=CH_2$	3,095–3,075	3·23– 3·25	m.	CH str.
	895– 885	11·17–11·30	s.	o.o.p. def.
	1,800–1,780	5·56– 5·62	m.	overtone
	1,420–1,410	7·04– 7·09	w.	CH_2 i.p. def.
$CR_1R_2=CHR_3$	3,040–3,010	3·29– 3·32	m.	CH str.
	850– 790	11·76–12·66	m.	CH o.o.p. def.

The $C=C$ stretching frequency is affected by both the mesomeric and inductive effects of substituents attached directly to the double bond. The $=CH_2$ out of plane deformation of the vinyl group is sensitive only to the mesomeric effect, whereas the $CH=CH$ trans CH deformation is relatively insensitive to the mesomeric effect but is affected by the inductive effects.

	$C=C$ str.	$=CH_2$ o.o.p. def.	$CH=CH$ def.
$CH_2=CHR$	*ca.* 1,640	*ca.* 910	*ca.* 990
$CH_2=CHCO.OR$	1,640–1,630	*ca.* 961	*ca.* 982
$CH_2=CHO.CO.R$	1,700–1,665	*ca.* 870	*ca.* 950
$CH_2=CHOR$	1,680–1,660	*ca.* 815	*ca.* 960
$CH_2=CHF$	*ca.* 1,650	*ca.* 860	*ca.* 925
$CH_2=CF_2$	1,755–1,735	*ca.* 800	—

During vibrations of the $C=C$ and $C=O$ groups of acyclic alkenes and ketones the carbon atoms directly attached to the multiple bond usually remain stationary, thereby localizing the vibration within the bond. However, the observed stretching frequency of the C=C bond of cyclic alkenes represents a coupled vibration of the C=C stretching mode with the stretching and bending modes of the adjacent C—C bond and therefore varies with the size of the ring. The minimum interaction occurs at a C=C—C angle of 90° when the C=C stretching vibration causes only bending of the attached C—C bond. At higher or lower angles C—C stretching also occurs as a result of the C=C stretching vibration. This increase in vibrational interaction produces an increase in the C=C stretching frequency. In acyclic systems the bond angles are usually invariant at *ca.* 120° and the interaction and consequently the position of the absorption band are fairly constant. For the cyclic compounds the wavelength of the C=C stretching vibration is directly related to $\cos^2\alpha$, where α is the C=C—C angle[5]. Hence, although the ring strain in cyclopropene and cyclohexene differ considerably, the positions of the observed C=C stretching bands are almost identical. Such a coincidence in the values would not have been predicted if the change in the stretching frequency was entirely dependent upon a change in the force constants, resulting from a rehybridization of the sp^2 orbitals[6].

Alkyl substitution of the alkene bond increases the C=C stretching frequency as further interaction can occur between the double bond and the C-alkyl bond, e.g. cyclopropene absorbs at 1,640 (6·10), 1,3,3,-trimethylcyclopropene at 1,765 (5·70), and 1,2,3,3,-tetramethylcyclopropene at 1,865 cm^{-1} (5·36 μ).

Similar arguments explain the increase in the frequencies of the C=O and C=C stretching vibrations of cyclic ketones (*Table 18*) and exocyclic alkenes with a decrease in the size of the rings.

Table 10. Cyclic and Exocyclic Alkenes

C—H *and* C=C *Stretching Vibrations*

*cyclo*propenes	*ca.* 3,080	*ca.* 3·25	*cyclo*heptenes	*ca.* 1,650	*ca.* 6·06
	ca. 1,640	*ca.* 6·10	*cyclo*octenes	*ca.* 1,675	*ca.* 5·97
*cyclo*butenes	*ca.* 3,060	*ca.* 3·27	exocyclic alkenes, $(CH_2)_nC=CH_2$		
	ca. 1,565	*ca.* 6·39			
*cyclo*pentenes	*ca.* 3,040	*ca.* 3·29	n = 2	*ca.* 1,780	*ca.* 5·62
	ca. 1,610	*ca.* 6·21	n = 3	*ca.* 1,680	*ca.* 5·95
*cyclo*hexenes	*ca.* 3,010	*ca.* 3·32	n = 4	*ca.* 1,660	*ca.* 6·02
	ca. 1,645	*ca.* 6·08	n = 5	*ca.* 1,650	*ca.* 6·06

Table 11. Alkynes and Allenes

Alkynes				
RC≡CH	3,340–3,300	2·99–3·03	m.	C—H str.
	2,140–2,100	4·67–4·76	w.	C≡C str.
$R_1C{\equiv}CR_2$	2,260–2,190	4·43–4·57	v.	C≡C str.
Allenes				
C=C=C	2,000–1;900	5·00–5·26	m.-s.	asym. CCC str.
	ca. 850	*ca.* 11·76	s.	CH_2 o.o.p. def.

AROMATIC HOMOCYCLIC AND HETEROCYCLIC COMPOUNDS

Table 12. Aromatic Homocyclic Compounds

Stretching Vibrations

=C—H str.	3,100–3,000	3·25–3·33	w.-m.	multiple peaks may appear in this region
C=C i.p. def	1,625–1,590	6·15–6·29	v.	usually close to 1,600 cm^{-1}
	1,590–1,570	6·29–6·37	v.	
	1,520–1,470	6·58–6·80	v.	usually close to 1,500 cm^{-1}
	1,465–1,430	6·83–6·99	v.	

Attempts have been made to rationalize the wide variations in the intensities of the ring vibrations in the 1,600–1,400 cm^{-1} region. It has been found that there is a general increase in the intensity of the bands, particularly of those near 1,600 cm^{-1}, as a result of charge disturbance within the ring through the electronic interaction between the ring and the substituents. More recent studies have correlated the square root of the integrated intensities of these bands with the σ_R^0 factors for the substituents[7]. The intensity of the 1,580 cm^{-1} band is considerably enhanced when the ring is conjugated with a carbonyl group.

The bands at 1,010, 992, and 606 cm^{-1} for unsubstituted benzene result from in-plane C—C deformation modes in which the carbon atoms move

C—H *In-plane Deformations and Benzene Ring Substitution*

monosubstitution	1,250–1,230	8·00–8·13	w.
	1,180–1,170	8·48–8·55	w.-m.
	1,160–1,150	8·62–8·70	w.
	1,080–1,065	9·26–9·39	m.
	1,030–1,025	9·71–9·76	w.-m.
1:2 disubstitution	1,290–1,250	7·75–8·00	w.
	1,180–1,150	8·48–8·70	w.-m.
	1,150–1,100	8·70–9·09	w.-m.
	1,055–1,010	9·48–9·90	m.
1:3 disubstitution	1,300–1,260	7·69–7·94	w.
	1,165–1,150	8·59–8·70	v.
	1,120–1,085	8·93–9·22	w.
	1,090–1,060	9·17–9·43	v.
1:4 disubstitution	1,300–1,265	7·69–7·91	w.-m.
	1,190–1,155	8·40–8·66	v.
	1,130–1,100	8·85–9·09	v.
	1,025–1,000	9·76–10·00	v.
1:2:3 trisubstitution	1,165–1,555	8·59–8·66	w.
	1,085–1,065	9·22–9·39	m.
	1,025–1,010	9·76–9·90	m.
1:2:4 trisubstitution	1,160–1,140	8·62–8·77	m.
	1,140–1,120	8·77–8·93	m.
	1,045–1,025	9·57–9·76	m.
1:3:5 trisubstitution	1,180–1,160	8·48–8·62	m.

radially or nearly so. For substituted benzenes these 'radial modes' can interact with the single bond stretching vibration of the attached substituent. Consequently these vibrations will be sensitive to the mass of the substituent. These bands have been termed 'X-sensitive bands'[8] and, in some instances, they can be used to characterize the X-substituent. Where this is so, mention of the band, which is usually to be found in the 1,300–1,050 cm^{-1} region, has been made in the relevant Tables.

In the case of monosubstituted and *meta*-disubstituted benzenes a 'radial mode' in which the carbon atoms 2, 4 and 6 move radially in phase and is therefore virtually insensitive to the mass of the substituent, is observed near 1,000 cm^{-1}. This vibration is called the ring breathing mode.

X-sensitive mode Ring breathing mode

C—H *Out-of-plane Deformations and Benzene Ring Substitution*

monosubstitution	900–860	11·11–11·63	w.-m.	5 adj. H atoms, l.v.
	770–730	12·99–13·70	s.	5 adj. H atoms
	710–690	14·08–14·49	s.	5 adj. H atoms
✓1:2 disubstitution	960–905	10·42–11·05	w.	4 adj. H atoms, l.v.
	850–810	11·76–12·35	w.	4 adj. H atoms, l.v.
	760–745	13·16–13·42	s.	4 adj. H atoms
1:3 disubstitution	960–900	10·42–11·11	m.	isolated H atom
	880–830	11·36–12·05	m.-s.	3 adj. H atoms
	820–790	12·20–12·66	w.-m.	3 adj. H atoms, l.v.
1:4 and 1:2:3:4 substitution	860–800 645	11·63–12·50	s.	2 adj. H atoms
1:2:3 trisubstitution	965–950	10·36–10·53	w.	3 adj. H atoms, l.v.
	900–885	11·11–11·30	w.	3 adj. H atoms, l.v.
	780–760	12·82–13·16	s.	3 adj. H atoms
	720–685	13·89–14·60	m.	3 adj. H atoms, l.v.
1:2:4 trisubstitution	940–920	10·64–10·87	w.	isolated H atom, l.v.
	900–885	11·36–11·30	m.	2 adj. H atoms
	780–760	12·82–13·16	s.	2 adj. H atoms
1:3:5 trisubstitution	950–925	10·53–10·81	v.	isolated H atom, l.v.
	860–830	11·49–12·05	s.	isolated H atom
1:2:3:5, 1:2:4:5, and 1:2:3:4:5 substitution	870–850	11·49–11·76	s.	isolated H atom

Benzene Ring Substitution Patterns of Summation Bands

Weak summation bands (overtones and combinations) of the CH out-of-plane deformation frequencies give absorption patterns in the range 2,000–1,650 cm^{-1} (5·00–6·06 μ), which are consistent and characteristic of the different substitutions of the benzene ring. Strong solutions are required to study these patterns [up to 20 times normal solution strengths (p. 23)]. Other bands occurring in this region, e.g. the strong C=C and C=O stretching fundamentals, mask the aromatic bands. Since the number of bands, their intensities and band shapes are more characteristic than absolute frequencies, no table is included here. These patterns are very useful in structural analysis and, though reference patterns are available[9], a preferred procedure is to prepare a set for each individual instrument.

Polycyclic Aromatic Compounds

Condensed ring systems absorb in similar regions to those observed for monocyclic aromatic compounds and, in general, the hydrogen substitution pattern for each ring may be considered separately. Thus, naphthalenes have two bands near 1,600 cm^{-1} (6·25) and bands in the ranges 1,520–1,505 (6·58–6·65) and 1,400–1,390 cm^{-1} (7·14–7·19 μ). 1-Substituted naphthalenes absorb in the regions 810–785 (12·35–12·74) and 780–760 cm^{-1} (12·82–13·16 μ) characteristic of three and four adjacent hydrogen atoms respectively, whilst 2-substituted naphthalenes absorb at 860–835 (11·63–11·98) (an isolated H atom), 835–805 (11·98–12·42) (two adjacent H atoms), and 760–735 cm^{-1} (13·16–13·61 μ) (four adjacent H atoms).

Anthracenes absorb in the range 1,640–1,620 (6·10–6·17) and near 1,550 cm^{-1} (6·45 μ) and may be differentiated from phenanthrenes which have two bands near 1,600 cm^{-1} (6·25 μ) and another band near 1,500 cm^{-1} (6·67 μ).

Table 13. Aromatic Heterocyclic Components: Six-membered Rings*

Pyridines and Related Compounds

Stretching Vibrations

Pyridines				
=C—H str.	3,095–3,010	3·23– 3·32	m.-s.	multiple peaks
C=C i.p. vib.	1,615–1,575	6·19– 6·35	v.	
	1,590–1,555	6·29– 6·43	v.	
	1,520–1,465	6·58– 6·83	v.	
	1,450–1,410	6·90– 7·09	v.	
	1,000– 990	10·00–10·10	m.	ring breathing vib.
Pyridinium Salts				
N^+—H str. (free)	3,340–3,210	2·99– 3·12	v.	multiple bands
(H bonded ion pair)	3,300–2,375	3·03– 4·21	v.	multiple bands
Pyridine 1-oxides				
=C—H str.	3,095–3,010	3·23– 3·32	m.-s.	multiple bands
C=C i.p. vib.	1,645–1,600	6·08– 6·25	v.	
	1,580–1,560	6·33– 6·41	v.	
	1,540–1,475	6·49– 6·78	v.	
	1,450–1,425	6·90– 7·02	v.	
	ca. 1,015	*ca.* 9·85	s.	ring breathing vib. 3-subst. only
N^+—O^- str.	1,310–1,220	7·64– 8·20	s.	

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* For a comprehensive survey and discussion of the spectra of heteroaromatic compounds, see reference 10. Characteristic substitution patterns in the region 2,000 – 1,650 cm^{-1} (5.00 – 6.06μ) have been observed for pyridines[11] and 2,2-bipyridyls[12]

Table 13—continued

C—H *In- and Out-of-plane Deformations and Ring Substitution*

2-monosubstitution	1,295–1,265	7·72– 7·90	w.	pyridines only
	1,150–1,145	8·70– 8·73	w.	pyridines and 1-oxides
	1,115–1,090	8·97– 9·17	w.	pyridines and 1-oxides
	1,055–1,040	9·48– 9·61	w.	pyridines and 1-oxides
	990– 960	10·10–10·42	m.	pyridine 1-oxides only
	780– 740	12·82–13·51	s.	pyridines only
3-monosubstitution	1,200–1,180	8·33– 8·48	v.	pyridines only
	1,160–1,155	8·62– 8·66	v.	pyridine 1-oxides only
	1,130–1,120	8·85– 8·93	w.	pyridines only
	1,120–1,080	8·93– 9·26	w.-m.	pyridine 1-oxides only
	1,110–1,100	9·01– 9·09	w.	pyridines only
	1,045–1,030	9·57– 9·71	w.	pyridines only
	980– 930	10·20–10·75	s.	pyridine 1-oxides only
	920– 890	10·87–11·24	w.	pyridines only
	820– 770	12·20–12·29	m.-s.	pyridines and 1-oxides
	730– 690	13·70–14·49		pyridines only
	680– 660	14·71–15·15	m.	pyridine 1-oxides only
4-monosubstitution	1,230–1,210	8·13– 8·26	v.	pyridines only
	1,175–1,165	8·51– 8·59	s.	pyridine 1-oxides only
	1,110–1,095	9·01– 9·13	w.	pyridine 1-oxides only
	1,070–1,065	9·35– 9·39	w.	pyridines only
	1,040–1,030	9·62– 9·71	m.	pyridine 1-oxides only
	850– 790	11·76–12·66	s.	pyridines and 1-oxides
2:3-disubstitution	815– 785	12·27–12·74		o.o.p. vib.
	740– 690	13·51–14·49	m.-s.	
2:5-disubstitution	825– 810	12·12–12·35		o.o.p. vib.
	735– 725	13·60–13·75		
2:6-disubstitution	815– 770	12·27–12·99		o.o.p. vib.
	750– 720	13·33–13·89		
3:4-disubstitution	890– 860	11·24–11·63	s.	pyridine 1-oxides only
	825– 810	12·12–12·35	s.	pyridine-1-oxides only
	860– 840	11·63–11·90	m.	pyridines only

Diazines and Triazines

Stretching Vibrations

=C—H str.	3,090–3,040	3·24–3·29	m.	
Pyrimidines	1,590–1,555	6·29–6·43	v.	
	1,565–1,520	6·39–6·58	v.	
	1,480–1,400	6·76–7·15	v.	
	1,410–1,375	7·09–7·28	v.	
	1,020– 990	9·80–10·10	m.	ring breathing vib.
Pyrazines and pyrazine 1-oxides	1,600–1,575	6·25–6·35	v.	
	1,550–1,520	6·45–6·58	w.-m.	
	1,500–1,465	6·67–6·83	m.-s.	
	1,420–1,370	7·04–7·30	m.-s.	
sym-Triazines	1,560–1,520	6·41–6·58	v.	
	1,490–1,450	6·71–6·90	v.	

Table 13—continued

Pyrylium Salts

Stretching Vibrations

=C—H str.	3,100–3,010	3·20– 3·32	w.-m.	multiple bands
C=C i.p. vib.	1,650–1,615	6·06– 6·19	vs.	
	1,560–1,520	6·41– 6·58	vs.	
	1,520–1,465	6·58– 6·83	m.	
	1,450–1,400	6·90– 7·14	v.	
	1,000– 970	10·00–10·31	v.	ring breathing vib.

C—H *Out-of-plane Deformations*

unsubstituted	*ca.* 960	*ca.* 10·42	s.	
	ca. 775	*ca.* 12·90	m.	o.o.p. ring vib.
2:6-disubstitution	*ca.* 935	*ca.* 10·70	m.	
	ca. 800	*ca.* 12·50	s.	
2:4:6-trisubstitution	960–900	10·42–11·11	v.	two bands. l.v.
	890–870	11·24–11·49	m.	
2:3:4:6-tetra-substitution	925–915	10·81–10·93	w.	l.v.
	900–880	11·11–11·36	w.	l.v.
2:3:5:6-tetra-substitution	710–700	14·08–14·29	m.	

Pyridones, Pyrones, and Related Compounds

Stretching Vibrations

Pyrid-2-ones and -thiones	1,670–1,655	5·99–6·04	vs.	C=O str.
	1,630–1,590	6·14–6·29	vs.	
	1,570–1,535	6·37–6·52	s.	
	1,500–1,470	6·67–6·80	m.	
	1,445–1,415	6·92–7·06	m.-s.	
	1,145–1,100	8·73–9·09	m.-s.	C=S str.
Pyrid-4-ones and -thiones	1,660–1,620	6·02–6·17	vs.	
	1,580–1,550	6·33–6·45	vs.	C=O str.
	1,515–1,485	6·60–6·74	w.-m.	
	1,470–1,400	6·80–7·14	m.-s.	
	1,120–1,105	8·93–9·05	vs.	C=S str.
Pyr-2-ones	1,735–1,730	5·76–5·78	s.	C=O str.
	1,650–1,635	6·06–6·12	m.	
	1,570–1,560	6·37–6·41	s.	
Pyr-4-ones and -thiones*	1,680–1,600	5·95–6·25	vs.	
	1,635–1,525	6·12–6·56	vs.	
	1,465–1,445	6·83–6·92	m.-s.	
	1,420–1,400	7·04–7·14	m.	
	ca. 1,100	*ca.* 9·09	s.	C=S str.

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* There is strong coupling of the C = O and C = C stretching vibrations such that no one band may be assigned to the C = O vibration. Thiapyrones and thiapyrthiones absorb at *ca.* 40 cm^{-1} lower frequency.

Table 14. Aromatic Heterocyclic Compounds: Five-membered Rings

Pyrroles

Stretching Vibrations

N—H str. (free bonded)	3,500–3,400	2·86–2·94	v.	
	3,400–3,000	2·94–3·23	s.	broad band
=C—H str.	3,100–3,000	3·23–3·33	m.	
C=C i.p. vib.	1,580–1,545	6·33–6·47	w.	two bands for 1-subst. pyrroles
	1,535–1,525	6·52–6·56	w.	1:2-, 1:2:5-, and 1:3:4-subst. pyrroles only
	1,500–1,475	6·66–6·78	m.-s.	1:2- subst. pyrroles only
	1,480–1,460	6·76–6·85	w.-m.	
	1,430–1,390	6·99–7·19	vs.	

N—H *and* C—H *In- and Out-of-plane deformations*

1-substitution	1,075–1,065	9·30– 9·39	s.	4 adj. H atoms
	1,035–1,015	9·66– 9·85	m.	4 adj. H atoms, l.v.
	930– 920	10·75–10·87	m.	4 adj. H atoms, l.v.
	725– 720	13·79–13·89	vs.	4 adj. H atoms
2-substitution	1,120–1,110	8·93– 9·01	w.-m.	N—H i.p. def.
	1,105–1,070	9·05– 9·35	m.-s.	3 adj. H atoms + NH. l.v.
	1,040–1,020	9·62– 9·80	m.-s.	3 adj. H atoms + NH. l.v.
	930– 925	10·75–10·81	w.	3 adj. H atoms + NH. l.v.
	885– 875	11·30–11·43	w.-m.	3 adj. H atoms + NH
1:2-disubstitution	1,095–1,085	9·13– 9·22	m.	3 adj. H atoms
	1,065–1,050	9·43– 9·52	v.	3 adj. H atoms
1:2:5-trisubstitution	1,040–1,030	9·62– 9·71	m.	2 adj. H atoms. l.v.
	980– 965	10·20–10·36	w.	2 adj. H atoms. l.v.
	760– 750	13·16–13·33	vs.	2 adj. H atoms
1:3:4-trisubstitution	1,060–1,050	9·43– 9·52	s.	isolated H atom
	935– 930	10·70–10·75	m.	isolated H atom
	780– 760	12·82–13·16	vs.	isolated H atom

Thiophens

Stretching Vibrations

=C—H	3,100–3,000	3·23– 3·33	m.	
C=C i.p. str.	1,555–1,480	6·43 –6·76	v.	
	1,445–1,390	6·92– 7·19	v.	
	1,375–1,340	7·28 –7·46	v.	
	1,240–1,195	8·06– 8·37	v.	
	840– 790	11·90–12·66	m.	ring breathing vib. 2-subst. cpds.
	895– 850	11·17–11·76	m.	ring breathing vib. 3-subst. cpds.

Table 14—continued

C—H *In- and Out-of-plane Deformations*

2-substitution	1,085–1,075	9·22– 9·30	w.	l.v.
	1,055–1,030	9·48– 9·71	w.-m.	
	940– 905	10·64–11·05	w.	
	865– 840	11·56–11·90	m.-s.	
3-substitution	1,100–1,070	9·09– 9·35	w.	l.v.
	ca. 1,155	*ca.* 8·66	w.	l.v.
	795– 745	12·58–13·42	s.	

Furans

Stretching Vibrations

=C—H str.	3,100–3,000	3·23– 3·33	m.	
C=C i.p. vib.	1,610–1,560	6·21– 6·41	v.	
	1,515–1,470	6·60– 6·80	v.	
	1,405–1,380	7·11– 7·25	v.	
	1,025–1,005	9·76– 9·95	m.-s.	ring breathing vib.

C—H *In- and Out-of-plane Deformations*

2-substitution	1,240–1,200	8·07– 8·33	v.	
	1,175–1,145	8·51– 8·73	m.-s.	
	1,085–1,070	9·22– 9·35	m.	
	945– 910	10·58–10·99	m.	
	890– 880	11·24–11·36	v.	
	840– 800	11·90–12·50	w.	l.v.
3-substitution	1,170–1,150	8·55– 8·70	s.	
	1,080–1,050	9·26– 9·52	m.-s.	
	1,025–1,005	9·76– 9·95	s.-vs.	
	ca. 920	*ca.* 10·87	v.	l.v.
	880– 870	11·36–11·49	s.	
	790– 720	12·66–13·89	s.	usually two bands

Azoles

The majority of azoles have four absorption bands in the ranges 1,670–1,520 (5·99–6·58), 1,555–1,470 (6·43–6·80), 1,490–1,390 (6·71–7·20), and 1,450–1,320 cm^{-1} (6·90–7·58 μ). Both the positions and the intensities of these bands vary considerably with the orientation of the ring heteroatoms and with the positions and type of the substituents. Although the out-of-plane CH deformation bands for these compounds may be correlated with the number and orientation of the aromatic hydrogen atoms they are of limited value.

Polycyclic Heteroaromatic Compounds

In general, the polycyclic compounds have between four and ten medium to strong bands in the 1,650–1,350 cm^{-1} (6·06–7·41 μ) region, which may be assigned to the aromatic in-plane ring deformations. It appears possible that the overall aromatic substitution pattern may be determined from the

CH deformation frequencies one would expect for the individual rings, e.g., 4-substituted quinolines absorb near 953 and 870 cm^{-1} (10·49–11·49 μ), characteristic of 4 adjacent hydrogen atoms, and near 850 cm^{-1} (11·76 μ), characteristic of 2 adjacent hydrogen atoms (cf. *Tables 12* and *13*).

ALCOHOLS, PHENOLS, ETHERS AND PEROXIDES

Table 15. Alcohols and phenols

O—H *Stretching Vibrations*					
free OH	3,670–3,580	2·73–2·79	v.	sharp band	
hydrogen bonded OH					
(a) intermolecular					
dimeric association	3,550–3,450	2·82–2·90	v.	sharp band	int. changes and frequency shifts on dilution
polymeric association	3,400–3,230	2·94–3·10	s.	broad band	
(b) intramolecular	3,590–3,420	2·79–2·92	v.	sharp band	unaffected by dilution
(c) chelate compounds	3,200–1,700	3·13–5·88	w.	very broad band	
(d) tropolones	*ca.* 3,100	*ca.* 3·23			
—OD	2,780–2,400	3·60–4·17	v.	O—D str.	
C—O *Stretching and* O—H *In-plane Deformations*					
primary alcohol	1,075–1,000	9·30–10·00	s.	l.v.	
	1,350–1,260	7·40– 7·94	s.	l.v.	
secondary alcohol	1,350–1,260	7·40– 7·94	s.	l.v.	
alkyl—CHOH	1,125–1,090	8·89– 9·17	s.	l.v.	
aryl—CHOH	1,075–1,000	9·30–10·00	s.	l.v.	
tertiary alcohol	1,410–1,310	7·09– 7·63	s.	l.v.	
	1,210–1,100	8·26– 9·09	s.	l.v.	
phenols	1,410–1,310	7·09– 7·63	s.	l.v.	
	1,260–1,180	7·94– 8·48	s.	l.v.	

Table 16. Ethers and Peroxides

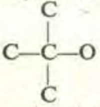
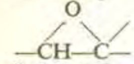
C—O *Stretching Vibrations*				
acyclic $CH_2—O—CH_2$	1,150–1,060	8·70– 9·43	s.	
 $C—\overset{\overset{C}{\vert}}{\underset{\underset{C}{\vert}}{C}}—O$	920– 800	10·87–12·50	s.	
aryl and aralkyl ethers	1,310–1,230	7·63– 8·13	s.	X-sensitive band
vinyl ethers	1,225–1,200	8·16– 8·33	s.	
epoxides	1,280–1,240	7·81– 8·07	s.	i.b.
epoxides (*trans*)	950– 860	10·53–11·63	v.	l.v.
epoxides (*cis*)	865– 785	11·56–12·74	m.	l.v.
trimethylene oxides	980– 970	10·20–10·31	s.	
higher cyclic ethers	1,140–1,070	8·77– 9·35	s.	l.v.
$—O—CH_2—O—$	*ca.* 940	*ca.* 10·65	s.	l.v.
phthalans	915– 895	10·93–11·17	m.	
acetals	1,180–1,040	8·48– 9·62	s.	several bands l.v.

Table 16—continued

C—H *Stretching Vibrations*

—O—CH$_3$	2,895–2,840	3·45– 3·52	m.	
	3,050–2,990	3·28– 3·34	w.	
alkyl acetals, —CH$_2$OCHROCH$_2$—	*ca.* 2,825	*ca.* 3·54	m.	
—O—CH$_2$—O—	*ca.* 2,780	*ca.* 3·60		
vinyl ethers	3,150–3,050	3·18– 3·28	w.	

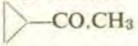
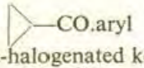
Peroxides, Hydroperoxides, and Peroxy Acids

all peroxy compounds	890– 830	11·24–12·05	w.	O—O str., l.v.
alkyl peroxides	1,150–1,030	8·70– 9·71	m.-s.	C—O str., l.v.
aryl peroxides	*ca.* 1,000	*ca.* 10·00	m.	X-sensitive band, l.v.
R.OOH	*ca.* 3,450	*ca.* 2·90	m.	O—H str.
acyl peroxides	1,820–1,810	5·50– 5·53	s.	C=O str.
	1,800–1,780	5·56– 5·62	s.	
aroyl peroxides	1,805–1,780	5·54– 5·62	s.	
	1,785–1,755	5·60– 5·70	s.	
peroxy acids	*ca.* 3,280	*ca.* 3·05	m.-s.	O—H str.
	ca. 1,760	*ca.* 5·68	s.	C=O str.
	ca. 1,175	*ca.* 8·51	m.-s.	C—O str.
	ca. 865	*ca.* 11·56	w.	O—O str.

KETONES AND ALDEHYDES

*Table 17. Ketones**†

C=O *Stretching Vibrations*

acyclic	1,725–1,700	5·80– 5·88	s.	
α:β unsat. acyclic compounds	1,700–1,685	5·88– 5·94	s.	s-cis, C=C vib. 1,625–1,615 cm^{-1}
	1,690–1,675	5·92– 5·97	s.	s-trans, C=C vib. 1,645–1,620 cm^{-1}
cross-conj. dienones	1,670–1,660	5·99– 6·02	s.	
aryl ketones	1,700–1,680	5·88– 5·95	s.	
diaryl ketones	1,670–1,660	5·99– 6·02	s.	
	1,705–1,680	5·86– 5·95	s.	
	1,695–1,670	5·90– 5·99	s.	
α-halogenated ketones†				
—CO—CO—	1,730–1,710	5·78– 5·85	s.	
—CO—CH$_2$—CO—				
(keto form)	*ca.* 1,700	*ca.* 5.88	v.	
(enol form)	1,640–1,535	6·10– 6·52	s.	chelated, broad peak
ortho CO.C$_6$H$_4$.OH (or NH$_2$)	1,655–1,610	6·04– 6·21	s.	H bonded
CO.CH$_2$CH$_2$.CO	1,725–1,705	5·80– 5·87	s.	
CO.O.CH$_2$.CO	1,745–1,725	5·73– 5·80	s.	

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* For influence of physical state and medium on frequency of carbonyl bands see Part I, p. 34.

† For ketones, except those in which hydrogen bonding occurs, additive shifts of the original C=O stretching frequencies, and hence of the range limits given in the table, are observed for α substituents, as opposite

Table 17—continued

Other Vibrations

CH_3—CO—	1,360–1,355	7·35–7·38	s.	CH_3 def.
—CH_2—CO—	1,435–1,405	6·97–7·12	s.	CH_2 def.
alkyl ketones	1,325–1,215	7·55–8·23	m.	l.v.
aryl ketones	1,225–1,075	8·17–9·30	m.	l.v.
C=O	3,550–3,200	2·82–3·13	w.	C=O str. overtones

α substituent	Frequency shift cm^{-1}	Wavelength shift μ	
α:β unsaturation	−30	+0·11	
α halogen	+20	−0·07	in cyclic ketones only equatorial halogen causes +20 cm^{-1} shift
αα′ halogens	+40	−0·15	
αα halogens	+20	−0·07	

Table 18. Cyclic Ketones

C=O *Stretching Vibrations*

9–7 membered rings	*ca.* 1,705	*ca.* 5·87	s.	
6 membered rings	*ca.* 1,720	*ca.* 5·81	s.	
5 membered rings	*ca.* 1,750	*ca.* 5·71	s.	
4 membered rings	*ca.* 1,790	*ca.* 5·59	s.	
ketenes ('2 membered ring')	2,150–2,120	4·56– 4·71	s.	
cyclopropenones	1,645–1,620	6·08– 6·17	s.	
	1,865–1,845	5·36– 5·42	s.	C=C str.
quinones—2 CO's in the same ring	1,690–1,655	5·92– 6·04	s.	
2 CO's in 2 rings	1,655–1,635	6·04– 6·12	s.	
tropones	1,600–1,575	6·25– 6·35	s.	
tropolones	1,620–1,600	6·17– 6·25	s.	H bonded

Table 19. Aldehydes

C=O *Stretching Vibrations*

sat. aliphatic aldehydes	1,740–1,720	5·75–5·81	s.	
α:β-unsat. aldehydes	1,705–1,685	5·78–5·93	s.	
conj. polyene aldehydes	1,680–1,660	5·95–6·02	s.	
aryl aldehydes	1,715–1,695	5·83–5·90	s.	
—C(OH)=C—CHO	1,670–1,645	5·99–6·08	s.	intramolecular H bonding

C—H *Stretching and Deformation Vibrations*

CHO	2,880–2,650	3·47– 3·77	w.-m.	C—H str. 2 bands may appear
	975– 780	10·26–12·82	w.	l.v.; C—H def.

Other Vibrations

aliphatic aldehydes	1,440–1,325	6·94–7·55	m.	l.v.
aryl aldehydes	1,415–1,350	7·07–7·41	m.	l.v.
	1,320–1,260	7·58–7·94	m.	l.v.
	1,230–1,160	8·13–8·62	m.	l.v.

CARBOXYLIC ACIDS AND DERIVATIVES

Table 20. Carboxylic Acids

O—H *Vibrations*				
free OH	3,550–3,500	2·82– 2·86	m.	O—H str.
bonded OH	3,300–2,500	3·00– 4·00	w.	broad band, O—H str.
all OH	955– 890	10·47–11·24	v.	o.o.p. def.
C=O *Stretching Vibrations*				
sat. aliphatic acids	1,725–1,700	5·80–5·88	s.	all acids examined as dimers in so. ph. or liq. ph.
α:β-unsat. acids	1,715–1,680	5·83–5·95	s.	
aryl acids	1,700–1,680	5·88–5·95	s.	
intramolecular H bonded acids	1,680–1,650	5·95–6·06	s.	
α-halogeno acids	1,740–1,715	5·75–5·83	s.	
Other Vibrations				
solid fatty acids	1,350–1,180	7·40–8·48	w.	CH_2 vib., characteristic band patterns
CO_2H	1,440–1,395	6·94–7·17	w.	combination band of C—O str. and OH i.p. def.
	1,320–1,210	7·58–8·26	s.	
carboxylate ion CO_2	1,610–1,550	6·21–6·45	s.	asym. str.
	1,420–1,300	7·04–7·69	m.	sym. str.

Table 21. Acid Halides and Anhydrides

C—O *Stretching Vibrations*				
anhydrides—cyclic	1,310–1,210	7·63–8·26	s.	
acyclic	1,175–1,045	8·51–9·57	s.	
C=O *Stretching Vibrations*				
'5' ring anhydrides	1,870–1,845	5·35– 5·42	s.	
	1,800–1,775	5·56– 5·63	s.	
conj. '5' ring anhydrides	1,860–1,850	5·38– 5·41	s.	
	1,780–1,760	5·62– 5·68	s.	
acyclic anhydrides	1,825–1,815	5·48– 5·51	s.	
	1,755–1,745	5·70– 5·73	s.	
conj. acyclic anhydrides	1,780–1,770	5·62– 5·65	s.	
	1,725–1,715	5·80– 5·83	s.	
alkyl acid chlorides	1,810–1,795	5·53– 5·57	s.	
aryl acid chlorides	1,785–1,765	5·60– 5·67	s.	

*Table 22. Esters and Lactones**

C=O *Stretching Vibrations*

sat. aliphatic esters	1,750–1,720	5·71– 5·81	s.	
α:β unsat. and aryl esters*	1,730–1,705	5·78– 5·86	s.	
enol acetates	1,760–1,745	5·68– 5·73	s.	
carbonates	*ca.* 1,740	*ca.* 5·75	s.	
α-keto esters and α-diesters	1,755–1,740	5·70– 5·75	s.	
enolic β-keto esters	1,655–1,635	6·04– 6·12	s.	chelation
o-hydroxy (amino) benzoates, etc.	1,690–1,670	5·92– 5·99	s.	chelation
γ-keto esters, non-enolic β-keto esters, and γ-(and higher) diesters	1,750–1,735	5·71– 5·76	s.	
β-lactones	*ca.* 1,825	*ca.* 5·48	s.	
γ-lactones	1,795–1,760	5·57– 5.68	s.	
δ-lactones	1,750–1,735	5·71– 5·76	s.	
α:β-unsat. γ-lactones	1,790–1,775	5·59– 5·63	s.	
	1,765–1,740	5·67– 5·75	s.	
β:γ-unsat. γ-lactones	1,805–1,785	5·54– 5·60	s.	

C—O *Stretching Vibrations* (*several bands*)

formates	1,200–1,160	8·33– 8·62	s.	
acetates	1,260–1,230	7·93– 8·13	s.	
propionates and higher esters	1,280–1,160	7·81– 8·62	s.	
carbonates	1,300–1,150	7·69– 8·70	s.	
esters of α:β unsat. aliphatic acids	1,330–1,160	7·52– 8·62	s.	
esters of aromatic acids	1,300–1,100	7·69– 9·09	s.	
enol acetates	1,220–1,200	8·20– 8·33	s.	

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* For α-substituted esters and lactones, other than those in which hydrogen bonding occurs, the following additive shifts of C=O stretching frequency (or wavelength) for individual compounds and range limits apply approximately:

α-substituent	Frequency shift cm^{-1}	Wavelength shift μ	
α:β double bond	−20	+0·07	
α-halogen	+20	−0·07	
αα-halogens	+20	−0·07	2 bands for soln. spec.

AMINES AND IMINES

Table 23. Amines and Imines

N—H *Stretching Vibrations*

primary amines	3,550–3,330	2·82– 3·00	v.	asym. str.
	3,450–3,250	2·90– 3·08	v.	sym. str.
secondary amines	3,500–3,300	2·86– 3·03	v.	
imines	3,400–3,300	2·94– 3·03	v.	l.v.
associated N—H	3,400–3,100	2·94– 3·23	m.	
free N—D	2,600–2,400	3·85– 4·15	v.	

Table 23—continued

N—H *Deformation Vibrations*

primary amines	1,650–1,580	6·06– 6·33	m.-s.	
secondary amines	*ca.* 1,500	*ca.* 6·67	w.	l.v.

C—N *Stretching Vibrations*

aliphatic amines:				
primary	1,090–1,070	9·17– 9·35	w.-m.	l.v.
secondary	1,190–1,130	8·40– 8·85	w.-m.	l.v.
aromatic amines:				
primary	1,330–1,250	7·52– 8·00	s.	X-sensitive band
secondary	1,340–1,260	7·46– 7·94	s.	
tertiary	1,380–1,330	7·25– 7·52	s.	

Other Vibrations

N-Methyl	2,820–2,760	3·55– 3·62	m.-s.	C—H str.

Table 24. Charged Amine Derivatives
(co-ordination complexes, amine hydrochlorides)

NH_3^+ *Stretching and Deformation Vibrations*

NH_3^+	*ca.* 3,380	*ca.* 2·96	m.	NH_3^+ str. } values for soln.
	ca. 3,280	*ca.* 3·05	m.	NH_3^+ str. } spectra only
	3,350–3,150	2·99–3·18	m.	NH_3^+ str., so. ph. spec., intermolecular H bonding, multiple bands may appear
	1,625–1,560	6·15– 6·41	m.	asym. NH_3^+ def.
	1,550–1,505	6·45– 6·65	m.	sym. NH_3^+ def.
	ca. 800	*ca.* 12·50	w.	NH_3^+ rocking

NH_2^+ *Vibrations*

NH_2^+	3,000–2,700	3·33– 3·70	s.	NH_2^+ str. vib.
	1,620–1,560	6·17–6·41	m.-s.	NH_2^+ def.
	ca. 800	*ca.* 12·50	w.	NH_2^+ rocking, l.v.

NH^+ *Vibrations*

$C=NH^+$	2,700–2,330	3·70– 4·29	s.	NH^+ str.
all NH^+	2,200–1,800	4·55–5·56	w.-m.	l.v., NH^+ str.

AMIDES, AMINO ACIDS AND RELATED COMPOUNDS

Table 25. Amides

NH *Stretching Vibrations*

primary amides:				
free NH	3,540–3,480	2·83– 2·88	s.	
	3,420–3,380	2·92– 2·96	s.	
bonded NH	3,360–3,320	2·97– 3·01	m.	
	3,220–3,180	3·11– 3·15	m.	
secondary amides:				
free NH (*cis*)	3,440–3,420	2·91– 2·93	s.	
free NH (*trans*)	3,460–3,440	2·89– 2·91	s.	
bonded NH (*cis*)	3,180–3,140	3·15– 3·19	m.	
bonded NH (*trans*)	3,330–3,270	3·00– 3·06	m.	
primary urethanes	3,450–3,200	2·90– 3·13	m.	
secondary urethanes:				
free NH	3,430–3,390	2·92– 2·95	m.	
bonded NH	*ca.* 3,300	*ca.* 3·03	m.	

NH *Deformation Vibrations*

H bonded secondary amides	*ca.* 700	*ca.* 14·3		o.o.p. def., int. falls on dilution. Amide V band

C=O *Stretching Vibrations* (Amide—I band)

primary amides	*ca.* 1,690	*ca.* 5·92	s.	dil. soln. spec.
	ca. 1,650	*ca.* 6·06	s.	so. ph. spec.
secondary amides	1,700–1,665	5·88– 6·01	s.	dil. soln. spec.
	1,680–1,630	5·95– 6·14	s.	so. ph. spec.
tertiary amides	1,670–1,630	5·99– 6·14	s.	dil. soln. or so. ph. spec.
simple β-lactams	1,760–1,730	5·68– 5·78	s.	dil. soln. spec.
ring-fused β-lactams	1,780–1,770	5·62– 5·65	s.	l.v., dil. soln. spec.
simple γ-lactams	*ca.* 1,700	*ca.* 5·88	s.	l.v.
ring-fused γ-lactams	1,750–1,700	5·71– 5·88	s.	
larger-ring cyclic lactams	*ca.* 1,680	*ca.* 5·95	s.	dil. soln. spec.
ureas,				
—NH—CO—NH—	*ca.* 1,660	*ca.* 6·02	s.	
—CO—NH—CO—	1,790–1,720	5·59– 5·81	s.	
	1,710–1,670	5·85– 5·99	s.	
urethanes	1,740–1,690	5·75– 5·92	s.	

Combination Bands of NH *Deformation and* C—N *Stretching Vibrations*

primary amides	1,650–1,620	6·06– 6·17	s.	so. ph. spec.	Amide II band
	1,620–1,590	6·17– 6·31	s.	dil. soln. spec.	
secondary acyclic amides	1,570–1,515	6·37– 6·60	s.	so. ph. spec.	
	1,550–1,510	6·45– 6·62	s.	dil. soln. spec.	
secondary amides	1,305–1,200	7·67– 8·33	m.	l.v., i.p. combination, Amide III	
urethanes	1,530–1,510	6·54– 6·62	s.	Amide II band	

Table 25—continued

Other Vibrations

primary amides	1,420–1,400	7·04– 7·14	m.	l.v.
secondary amides	770– 620	13·00–16·13	m.	l.v., Amide IV band
	630– 530	15·87–18·87	s.	l.v., Amide VI band
urethanes	1,350–1,250	7·41– 8·00	m.-s.	C—N—C=O vib. l.v.
	1,200–1,050	8·33– 9·52	m.-s.	CO.O vib., several bands l.v.

Table 26. Amino-acids, Amido-acids and Related Ionic Molecules

Amino-acids

amino-acids containing an NH_2 group	3,100–2,600	3·23– 3·85	m.	NH_3^+ str.
	1,665–1,585	6·01– 6·31	w.	NH_3^+ def. Amino-acid I band
	1,550–1,485	6·45–6·73	v.	NH_3^+ def. Amino-acid II band
dicarboxylic α-amino-acids	1,755–1,720	5·70–5·81	s.	C=O str., unionized carboxyl
other dicarboxylic amino-acids	1,730–1,700	5·78–5·88	s.	
dicarboxylic amino-acids	1,230–1,215	8·13–8·23	s.	C—O vib.
all amino acids	1,600–1,560	6·25–6·41	s.	ionized carboxyl, C=O str.
	2,760–2,530	3·62–3·95	w.	i.b., l.v.
	2,140–2,080	4·67–4·81	w.	NH_3^+ str., i.b., l.v.
	1,335–1,300	7·49–7·70	m.	i.b.

Amino-acid Salts $H_2N—(C)_n—CO_2^-M^+$

NH_2	3,400–3,200	2·94–3·13	m.	2 bands, NH_2 str.
CO_2^-	1,600–1,560	6·25–6·41	s.	ionized carboxyl C=O str.

Amino-acid Hydrochlorides $H_3N^+—(C)_n—CO_2H\ Cl^-$

NH_3^+	3,130–3,030	3·20–3·30	m.	NH_3^+ str., i.b.
	1,610–1,590	6·21–6·29	w.	NH_3^+ def.
	1,550–1,485	6·45–6·73	v.	NH_3^+ def.
α-amino-acid hydrochlorides	1,755–1,730	5·70–5.78	s.	C=O str.
other amino-acid hydrochlorides	1,730–1,700	5·78–5·88	s.	C=O str.
all amino-acid hydrochlorides	3,030–2,500	3·30– 4·0	w.	series of nearly continuous bands
	ca. 2,000	*ca.* 5·0	w.	
	1,335–1,300	7·49–7·70	m.	
	1,230–1,215	8·13–8·23	s.	C—O vib.

Amido-acids

NH	3,390–3,260	2·95–3·07	m.	N—H str.
α-amido-acids	1,725–1,695	5·80–5·90	s.	C=O str. (acid)
most amido-acids	2,640–2,360	3·79–4·24	w.	ib., l.v.
	1,945–1,835	5·14–5·45	w.	
α-amido-acids	1,620–1,600	6·14–6·25	s.	Amide I band
other amido-acids	1,650–1,620	6·06–6·14	s.	Amide I band
all amido-acids	1,570–1,500	6·37–6·67	s.	Amido II band
	1,230–1,215	8·13–8·23	s.	C—O vib.

NON-AROMATIC UNSATURATED NITROGEN AND NITROGEN–OXYGEN COMPOUNDS

Table 27. Non-aromatic Unsaturated Nitrogen Compounds

$C=N$ *Stretching Vibrations*

aliphatic azomethenes	1,670–1,665	5·99– 6·01	w.	
aryl azomethenes	1,670–1,650	5·99– 6·06	w.-m.	
α:β unsat. azomethenes	1,660–1,635	6·02– 6·12	m.	
oximes	1,690–1,620	5·92– 6·17	w.-m.	
isoureas	1,670–1,655	5·99– 6·04	m.	
amidines	1,685–1,580	5·93– 6·33	s.	
guanidines	1,670–1,500	5·99– 6·67	v.	
cyclic α:β unsat. $C=N$	1,660–1,560	6·02– 6·41	v.	e.g. pyrrolines

$A=B=N$ *Allenic-type Stretching Vibrations*

$N=C=N$	2,155–2,130	4·64– 4·70	vs.	carbodiimides
$N=C=O$	2,275–2,240	4·40– 4·46	vs.	isocyanates
$[R—C=N=N]^+$	2,310–2,135	4·33– 4·47	s.	diazonium salts
$—N=N=N$	2,160–2,120	4·63– 4·72	s.	azides, asym. str.
	1,300–1,275	7·69– 7·84	w.	azides, l.v., sym. str.

$C\equiv N$ *Stretching Vibrations*

sat. nitriles	2,260–2,240	4·43– 4·46	w.-m.	
acyclic α:β-unsat. nitriles	2,235–2,215	4·47– 4·52	s.	
aryl nitriles	2,240–2,220	4·46– 4·51	m.-s.	
isonitriles	2,145–2,135	4·66– 4·47	s.	l.v.
aryl isonitriles	2,125–2,110	4·71– 4·74	s.	l.v.

$N=N$ *Stretching Vibrations*

alkyl azo compounds	1,570–1,555	6·37– 6·43	v.	
α:β unsat. compounds	*ca.* 1,500	*ca.* 6·67	v.	l.v.
unsymmetric aromatic *trans* azo compounds	*ca.* 1,420	*ca.* 7·04		l.v.
cis compounds	*ca.* 1,510	*ca.* 6·62		l.v.

Table 28. Covalent Compounds Containing Nitrogen–Oxygen Bonds

Oximes $R_2C=NOH$

$—NOH$	3,650–3,500	2·74– 2·86	v.	free O—H str.
	3,300–3,150	3·03– 3·18	v.	bonded O—H str.
	1,690–1,620	5·92– 6·17	m.-w.	$C=N$ str.
	ca. 930	*ca.* 10.75		N—O str.

Table 28—continued

NO_2 *Vibrations, etc.—Nitro Compounds* ($R{\cdot}NO_2$)

alkyl nitro compounds	998– 914	10·02–10·94	m.-s.	C—N str. (*trans*) l.v.
primary and secondary nitro	917– 875	10·91–11·43	m.-s.	C—N str. (*gauche*) l.v.
	1,565–1,545	6·39– 6·47	s.	asym. NO_2 str.
	1,385–1,360	7·22– 7·35	s.	sym. NO_2 str.
	1,380	7·25	m.	CH_2 def. in $—CH_2—NO_2$
	655– 605	15·27–16·53	vs.	NO_2 def.
tertiary nitro	1,545–1,530	6·47– 6·54	s.	asym. NO_2 str.
	1,360–1,340	7·35– 7·46	s.	sym. NO_2 str.
α:β-unsat. nitro	1,530–1,510	6·54– 6·62	s.	asym. NO_2 str.
	1,360–1,335	7·35– 7·49	s.	sym. NO_2 str.
α-halogeno nitro	1,580–1,570	6·33– 6·37	s.	asym. NO_2 str.
	1,355–1,340	7·38– 7·46	s.	sym. NO_2 str.
α:α dihalogenonitro	1,600–1,575	6·25– 6·35	s.	asym. NO_2 str.
	1,340–1,325	7·46– 7·55	s.	sym. NO_2 str.
aromatic nitro	1,550–1,510	6·45– 6·62	s.	asym. NO_2 str.
	1,365–1,335	7·33– 7·49	s.	sym. NO_2 str.
	860– 840	11·63–11·90	s.	C—N vib., l.v.
	ca. 750	*ca.* 13·33	s.	i.b., l.v.

NO_2 *Vibrations—Covalent Nitrates* ($R{\cdot}O{\cdot}NO_2$)

NO_2	1,655–1,610	6·04–6·21	s.	asym. NO_2 str.
	1,300–1,255	7·69–7·97	s.	sym. NO_2 str.
	870– 855	11·49–11·70	s.	N—O str.
	760– 745	13·16–13·42	m.	NO_2 o.o.p. def.
	710– 695	14·08–14·39	m.	NO_2 def.

NO_2 *Vibrations—Nitramines* ($R_2N{\cdot}NO_2$)

sat. nitramines	1,585–1,530	6·31– 6·54	s.	asym. NO_2 str.
alkyl nitroguanidines	1,640–1,605	6·10– 6·23	s.	asym. NO_2 str.
aryl nitroguanidines and nitroureas	1,590–1,575	6·29– 6·35	s.	asym. NO_2 str.
all nitramines	1,300–1,260.	7·69– 7·94	s.	sym. NO_2 str.
	790– 770	12·66–12·99	m.	l.v.

NO *Vibrations—Nitroso Compounds* ($R{\cdot}NO$)

Aliphatic monomer	1,620–1,540	6·17– 6·49	s.	
Aromatic monomer	1,515–1,490	6·60– 6·71	s.	
Aliphatic dimer	1,420–1,330	7·04– 7·52	s.	*cis* dimer
	1,345–1,320	7·43– 7·58	s.	
	1,290–1,175	7·75– 8·50	s.	*trans* dimer
Aromatic dimer	*ca.* 1,409	*ca.* 7·10	s.	*cis.* dimer
	1,400–1,390	7·14– 7·19	s.	
	1,300–1,250	7·69– 8·00	s.	*trans* dimer

NO *Vibrations—Nitrites* (R—O—N=O)

R—O—N=O *trans* form	1,680–1,650	5·95– 6·06	vs.	N=O str.
cis form	1,625–1,610	6·16– 6·21	vs.	N=O str.
R—O—N=O *trans* form	815– 750	12·27–13·33	s.	N—O str., l.v.
cis form	850– 810	11·76–12·35	s.	N—O str., l.v.
R—O—N=O *cis* form	690– 615	14·49–16·26	s.	O—N=O def., l.v.
trans form	625– 565	16·00–17·70	s.	O—N=O def., l.v.
R—O—N=O	3,360–3,220	2·98– 3·11	m.	N=O str. overtones

Table 28—continued

NO *Vibrations—Nitrosamines* ($R_2N{\cdot}N{=}O$)

N—N=O	1,500–1,480	6·67–6·76	s.	N=O str., vap. ph. spec.
	1,460–1,440	6·85–6·94	s.	N=O str., dil. soln. spec.
	ca. 1,050	*ca.* 9·52	s.	N—N str., l.v.
	ca. 660	*ca.* 15·15	s.	N—N=O def., l.v.

NO *Vibrations—Amine Oxides* ($R_3N^+{-}O^-$)

pyridine and pyrimidine N-oxides	1,310–1,220	7·64– 8·20	m.-s.	N—O str., frequency varies widely with ring substituents
	895– 840	11·17–11·90	m.	N—O def.
tert. aliphatic N-oxides	970– 950	10·31–10·53	s.	N—O str., l.v.
aryl nitrile N-oxides	*ca.* 1,370	*ca.* 7·30	s.	N—O str., l.v.

NO *Vibrations—Azoxy Compounds* ($R{\cdot}N{:}N^+{-}O^-{\cdot}R$)

Aromatic compounds	1,480–1,450	6·76– 6·90	m.-s.	asym. N=N—O
	1,335–1,315	7·49– 7·60	m.-s.	sym. N=N—O
Aliphatic compounds	1,530–1,495	6·54– 6·69	m.-s.	

ORGANO-HALOGEN AND ORGANO-SULPHUR COMPOUNDS

Table 29. Organo-Halogen Compounds

Aliphatic C—X *Stretching Vibrations*

C—F monofluorinated compounds	1,110–1,000	9·01–10·00	s.	
C—F difluorinated compounds	1,250–1,050	8·00– 9·50	vs.	2 bands
C—F polyfluorinated compounds	1,400–1,100	7·14– 9·10	vs.	multiple bands
CF_3—CF_2	1,365–1,325	7·33– 7·55	s.	
C—Cl monochlorinated compounds*—primary	730– 650	13·70–15·38	s.	
secondary	675– 610	14·81–16·39	s.	
tertiary	630– 560	15·87–17·86	s.	
C—Cl equatorial	780– 750	12·80–13·33	s.	
C—Cl axial	730– 580	13·70–17·25	s.	
C—Cl polychlorinated compounds	800– 700	12·50–14·30	vs.-s.	l.v.
C—Br*	680– 515	14·71–19·42	s.	
C—Br equatorial	750– 700	13·33–14·29	s.	
C—Br axial	690– 550	14·50–18·20	s.	
C—I	600– 500	16·67–20·00	s.	l.v.

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* Frequency of the band depends upon the geometrical conformation of the molecule. *Trans* isomers absorb at a higher frequency than *gauche* isomers.

Table 29—continued

C—X *Deformation Vibrations*

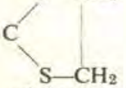
CF_3	1,350–1,120	7·41– 8·93	s.	
	780– 680	12·82–14·71		
CF_2	1,280–1,120	7·81– 8·93	s.	
$CF—CF_3$	745– 730	13·42–13·70	s.	
$C{=}CF_2$	1,755–1,735	5·70– 5·76		C=C str.
$CF{=}CF_2$	1,800–1,780	5·55– 5·62		C=C str.
	1,340–1,300	7·46– 7·69	s.	

Aromatic C—X *Stretching Vibrations* (X-Sensitive Band)

Fluoro compounds	1,270–1,100	7·88– 9·09	m.-s.	
Chloro compounds	1,105–1,035	9·05– 9·66	m.-s.	
Bromo compounds	1,090–1,025	9·18– 9·76	m.-s.	
Iodo compounds	*ca.* 1,060	*ca.* 9·43	m.-s.	

Table 30. Organo-Sulphur Compounds

C—S *Stretching Vibrations*

alkyl—S	705– 570	14·18–17·54	w.	l.v.
	745– 650	13·42–15·38	w.	l.v. several bands
α:β unsat. compounds	*ca.* 740	*ca.* 13·51	v.	
aryl—S	1,110–1,070	9·01– 9·35	m.	X-sensitive band
—CS·S·S·CS—	690– 685	14·49–14·60		l.v.

C=S *Stretching Vibrations*

thioesters	1,225–1,175	8·16– 8·51	s.	
thioureas and thioamides	1,210–1,045	8·26– 9·67	s.	bands resulting from coupling with C—N vib. also found near 1,500 cm^{-1}
$(RS)_2C{=}S$	1,060–1,050	9·43– 9·52	s.	
$(RO)_2\ C{=}S$	1,235–1,210	8·10– 8·26	s.	
$(aryl)_2\ C{=}S$	1,225–1,210	8·17– 8·26	s.	
$—C{=}C—C{=}S$	1,155–1,140	8·66– 8·77	s.	
pyrothiones and pyridthiones	1,140–1,110	8·77– 9·01	s.	

S—H *Stretching Vibrations*

	2,590–2,550	3·86–3·92	w.	

Table 30—continued

Other Vibrations

S—CH$_3$	2,990–2,955	3·34– 3·39	m.-s.	
	2,900–2,865	3·45– 3·49	m.-s.	
	1,440–1,415	6·94– 7·06	m.	
	1,330–1,290	7·52– 7·75	m.-s.	

S=O *Stretching Vibrations*

sat. or unsat. sulphoxides	1,070–1,030	9·35– 9·71	s.	so. ph. spec. 10–20 cm^{-1} lower
(RO)$_2$SO, sulphites	1,220–1,170	8·20– 8·55	s.	
R·SO·OR, sulphinic esters	1,140–1,125	8·77– 8·89	s.	
R·SO·OH, sulphinic acids	1,090– 990	9·17–10·10	s.	
R$_2$SO$_2$, sat. or unsat. sulphones	1,350–1,290	7·41– 7·75	vs.	so. ph. spec. 10–20 cm^{-1} lower
	1,165–1,120	8·59– 8·93	vs.	
R·SO$_2$OH, anhydrous sulphonic acids	1,350–1,340	7·41– 7·46	s.	
	1,165–1,150	8·59– 8·70	s.	S—O str.
	910– 895	10·99–11·17		
hydrated sulphonic acids and RSO$_3^-$, ionic sulphonates	1,230–1,120	8·13– 8·93	s.	
	1,080–1,025	9·26– 9·76	s.	
R·SO$_2$OR, covalent sulphonates	1,420–1,330	7·04– 7·52	s.	
	1,200–1,145	8·33– 8·73	s.	
(RO)$_2$SO$_2$, covalent sulphates	1,440–1,350	6·94– 7·41	s.	
	1,230–1,150	8·13– 8·70	s.	
RSO$_2$Cl, sulphonyl chlorides	1,390–1,340	7·19– 7·46	s.	
	1,190–1,160	8·40– 8·62	s.	
RSO$_2$F, sulphonyl fluorides	1,410–1,400	7·09– 7·14	s.	
	1,210–1,200	8·26– 8·33	s.	so. ph. spec. 10–20 cm^{-1} lower
RSO$_2$NR$_2$, sulphonamides	1,380–1,325	7·25– 7·55	vs.	
	1,180–1,140	8·48– 8·77	vs.	
	950– 860	10·53–11·63	m.	

PHOSPHORUS, SILICON AND BORON COMPOUNDS

Table 31. Organo-Phosphorus Compounds

P—C *Vibrations, etc.*

P—CH$_3$	1,430–1,390	6·99– 7·19	m.-s.	asym. CH$_3$ def.
	1,300–1,275	7·69– 7·85	m.-s.	sym. CH$_3$ def.
	980– 890	10·20–11·24	s.	CH$_3$ def.
	790– 770	12·66–12·99	s.	P—C str.
P—CH$_2$	780– 760	12·82–13·16	s.	P—C str.
P—CH$_2$ (benzyl)	795– 740	12·58–13·51	s.	P—C str.
P—aryl	1,115–1,090	8·97– 9·17	s.	X-sensitive band
	725– 705	13·79–14·18	s.	X-sensitive band

P—H *Vibrations*

P—H str.	2,450–2,270	4·08– 4·41	m.	
P—D str.	1,795–1,650	5·57– 6·06	m.	

Table 31—continued

P—O *Vibrations, etc.*

P—OH	2,700–2,560	3·70– 3·90	w.	OH str., broad band, strong H bonding
	1,040– 910	9·62–10·99	s.	P—O str.
all P—O-alkyls	1,050– 970	9·52–10.31	vs.	asym. P—O—C str.
P—O— methyl	1,190–1,170	8·40– 8·55	w.	CH_3 def.
P—O— ethyl	1,165–1,155	8·59– 8·68	w.	
P—O— aryl	1,260–1,160	7·94– 8·62	s.	X-sensitive band
	995– 915	10·05–10·93		pentavalent P—O str.
	875– 855	11·43–11·70		trivalent P—O str.
P—O—P	1,000– 870	10·00–11·49	s.	asym. str.
P=O (free)	1,350–1,175	7·41– 8·51	s.	P=O str.
P=O (H bonded)	1,250–1,150	8·00– 8·70	vs.	P=O str.

Table 32. Organo-Silicon Compounds

Si—C *Vibrations*

Si $(CH_3)_n$	1,280–1,255	7·81– 7·97	vs.	sym. CH_3 def.
n=1	*ca.* 765	*ca.* 13·07	vs.	Si—C str. and CH_3 def.
n=2	*ca.* 855	*ca.* 11·70	vs.	
	ca. 800	*ca.* 12·50	vs.	
n=3	*ca.* 840	*ca.* 11·90	vs.	
	ca. 765	*ca.* 13·07	vs.	
Si-phenyl	1,430–1,425	6·99– 7·02	vs.	ring vib.
	1,135–1,090	8·81– 9·17	vs.	X-sensitive band

Si—H *Vibrations*

Si—H str.	2,280–2,080	4·39– 4·81	vs.	
Si—H def.	950– 800	10·53–12·50		

Si—O *Stretching Vibrations*

Si—O—Si and Si—O—C	1,090–1,020	9·17– 9·80	vs.	Si—O str.

Table 33. Boron Compounds

BH	2,565–2,480	3·90– 4·03		BH str.
	1,180–1,110	8·48– 9·01		i.p. def.
	920– 900	10·87–11·11		o.o.p. def.
BH_2	2,640–2,570	3·79– 3·89	s.	sym. str.
	2,530–2,490	3·95– 4·02	s.	asym. str.
	1,170–1,140	8·55– 8·77	m.-s.	i.p. def.
	940– 920	10·64–10·87	m.	o.o.p. def.
B—H · · · · B	1,990–1,850	5·02– 5·40	w.	several bands
	1,610–1,540	6·21– 6·49	s.	
B—CH_3	1,460–1,405	6·85– 7·12	m.	CH_3 sym. def.
	1,320–1,280	7·58– 7·81	m.	CH_3 asym. def.
B—aryl	1,440–1,430	6·94– 6·99	m.-s.	ring. vib.
	1,280–1,220	7·81– 8·20	m.	X-sensitive band
B—O	1,350–1,310	7·41– 7·63	s.	B—O str.
B—N	1,465–1,330	6·83– 7·52	s.	B—N str.
B—Cl (alkylphenyl chloroborinates)	910– 890	10·99–11·24	s.	B—Cl str.

INORGANIC IONS, Etc.

Table 34. Inorganic Ions, Etc.

AsO_4^{3-}	*ca.* 800	*ca.* 12·50	s.	
AsF_6^-	705– 690	14·18–14·49	vs.	
BH_4^-	2,400–2,200	4·17– 4·55	s.	1 or more bands
	1,130–1,040	8·85– 9·62	s.	
BF_4^-	*ca.* 1,060	*ca.* 9·43	vs.	
	ca. 1,030	*ca.* 9·71	vs.	
BrO_3^-	810– 790	12·35–12·66	vs.	
CO_3^{2-}	1,450–1,410	6·90– 7·09	vs.	
	880– 800	11·36–12·50	m.	
HCO_3^-	1,420–1,400	7·04– 7·14	s.	
	1,000– 990	10·00–10·10	s.	
	840– 830	11·90–12·05	s.	
	705– 695	14·18–14·39	s.	
ClO_3^-	980– 930	10·20–10·75	vs.	
ClO_4^-	1,140–1,060	8·77– 9·43	vs.	broad absorption
CrO_4^{2-}	950– 800	10·53–12·50	s.	complex strong bands
$Cr_2O_7^{2-}$	950– 900	10·35–11·11	s.	
CN^-, CNO^-, and CNS^-	2,200–2,000	4·55– 5·00	s.	
CO	2,100–2,000	4·76– 5·00	s.	normal carbonyls
	ca. 1,830	*ca.* 5·46	s.	bridged carbonyls
HF_2^-	*ca.* 1,450	*ca.* 6·90	s.	
	ca. 1,230	*ca.* 8·13	s.	
IO_3^-	800– 700	12·50–14·29	s.	complex strong bands
MnO_4^-	920– 890	10·87–11·24	vs.	
	850– 840	11·76–11·90	m.	
NH_4^+	3,335–3,030	3·00– 3·30	vs.	
	1,485–1,390	6·73– 7·19	s.	
N_3^-	2,170–2,080	4·61– 4·81	s.	
	1,375–1,175	7·27– 8·51	w.	
NO_2^-	1,400–1,300	7·14– 7·69	s.	2 bands in complex nitrites
	1,250–1,230	8·00– 8·13	vs.	
	840– 800	11·90–12·50	w.	
NO_3^-	1,410–1,340	7·09– 7·46	vs.	
	860– 800	11·63–12·50	m.	
NO_2^+	1,410–1,370	7·09– 7·30	s.	
NO^+	2,370–2,230	4·22– 4·48	s.	
NO^+ (coordination comps.)	1,940–1,630	5·16– 6·14	s.	
NO^- (coordination comps.)	1,170–1,045	8·55– 9·57	s.	
NO (nitrosyl halides)	1,850–1,790	5·41– 5·59	s.	
PF_6^-	850– 840	11·76–11·90	vs.	
PO_4^{3-}, HPO_4^{2-}, and $H_2PO_4^-$	1,100– 950	9·09–10·53	s.	
$S_2O_3^{2-}$	1,660–1,620	6·02– 6·17	w.	
	1,000– 990	10·00–10·10	s.	
SO_4^{2-}	1,130–1,080	8·85– 9·26	vs.	
	680– 610	14·71–16·40	m.	
HSO_4^-	1,180–1,160	8·84– 8·62	s.	
	1,080–1,000	9·26–10·00	s.	
	880– 840	11·36–11·90	s.	
SO_3^{2-}	*ca.* 1,100	*ca.* 9·09	v.	l.v.
SeO_4^{2-}	*ca.* 830	*ca.* 12·05	s.	
SiF_6^{2-}	*ca.* 725	*ca.* 13·79	s.	
all silicates	1,100– 900	9·09–11·11	s.	
UO_2^{2+}	940– 900	10·64–11·11	s.	

RECIPROCALS

SUBTRACT

	0	1	2	3	4	5	6	7	8	9	1	2	3	4	5	6	7	8	9
1·0	1·0000	·9901	·9804	·9709	·9615	·9524	·9434	·9346	·9259	·9174	9	18	27	36	45	55	64	73	82
1·1	·9091	·9009	·8929	·8850	·8772	·8696	·8621	·8547	·8475	·8403	8	15	23	30	38	45	53	61	68
1·2	·8333	·8264	·8197	·8130	·8065	·8000	·7937	·7874	·7813	·7752	6	13	19	26	32	38	45	51	58
1·3	·7692	·7634	·7576	·7519	·7463	·7407	·7353	·7299	·7246	·7194	5	11	16	22	27	33	38	44	49
1·4	·7143	·7092	·7042	·6993	·6944	·6897	·6849	·6803	·6757	·6711	5	10	14	19	24	29	33	38	43
1·5	·6667	·6623	·6579	·6536	·6494	·6452	·6410	·6369	·6329	·6289	4	8	13	17	21	25	29	33	38
1·6	·6250	·6211	·6173	·6135	·6098	·6061	·6024	·5988	·5952	·5917	4	7	11	15	18	22	26	29	33
1·7	·5882	·5848	·5814	·5780	·5747	·5714	·5682	·5650	·5618	·5587	3	7	10	13	16	20	23	26	30
1·8	·5556	·5525	·5495	·5464	·5435	·5405	·5376	·5348	·5319	·5291	3	6	9	12	15	18	20	23	26
1·9	·5263	·5236	·5208	·5181	·5155	·5128	·5102	·5076	·5051	·5025	3	5	8	11	13	16	18	21	24
2·0	·5000	·4975	·4950	·4926	·4902	·4878	·4854	·4831	·4808	·4785	2	5	7	10	12	14	17	19	21
2·1	·4762	·4739	·4717	·4695	·4673	·4651	·4630	·4608	·4587	·4566	2	4	7	9	11	13	15	17	20
2·2	·4545	·4525	·4505	·4484	·4464	·4444	·4425	·4405	·4386	·4367	2	4	6	8	10	12	14	16	18
2·3	·4348	·4329	·4310	·4292	·4274	·4255	·4237	·4219	·4202	·4184	2	4	5	7	9	11	13	14	16
2·4	·4167	·4149	·4132	·4115	·4098	·4082	·4065	·4049	·4032	·4016	2	3	5	7	8	10	12	13	15
2·5	·4000	·3984	·3968	·3953	·3937	·3922	·3906	·3891	·3876	·3861	2	3	5	6	8	9	11	12	14
2·6	·3846	·3831	·3817	·3802	·3788	·3774	·3759	·3745	·3731	·3717	1	3	4	6	7	8	10	11	13
2·7	·3704	·3690	·3676	·3663	·3650	·3636	·3623	·3610	·3597	·3584	1	3	4	5	7	8	9	11	12
2·8	·3571	·3559	·3546	·3534	·3521	·3509	·3497	·3484	·3472	·3460	1	2	4	5	6	7	9	10	11
2·9	·3448	·3436	·3425	·3413	·3401	·3390	·3378	·3367	·3356	·3344	1	2	3	5	6	7	8	9	10
3·0	·3333	·3322	·3311	·3300	·3289	·3279	·3268	·3257	·3247	·3236	1	2	3	4	5	6	7	9	10
3·1	·3226	·3215	·3205	·3195	·3185	·3175	·3165	·3155	·3145	·3135	1	2	3	4	5	6	7	8	9
3·2	·3125	·3115	·3106	·3096	·3086	·3077	·3067	·3058	·3049	·3040	1	2	3	4	5	6	7	8	9
3·3	·3030	·3021	·3012	·3003	·2994	·2985	·2976	·2967	·2959	·2950	1	2	3	4	4	5	6	7	8
3·4	·2941	·2933	·2924	·2915	·2907	·2899	·2890	·2882	·2874	·2865	1	2	3	3	4	5	6	7	8
3·5	·2857	·2849	·2841	·2833	·2825	·2817	·2809	·2801	·2793	·2786	1	2	2	3	4	5	6	6	7
3·6	·2778	·2770	·2762	·2755	·2747	·2740	·2732	·2725	·2717	·2710	1	2	2	3	4	5	5	6	7
3·7	·2703	·2695	·2688	·2681	·2674	·2667	·2660	·2653	·2646	·2639	1	1	2	3	4	4	5	6	6
3·8	·2632	·2625	·2618	·2611	·2604	·2597	·2591	·2584	·2577	·2571	1	1	2	3	3	4	5	5	6
3·9	·2564	·2558	·2551	·2545	·2538	·2532	·2525	·2519	·2513	·2506	1	1	2	3	3	4	4	5	6
4·0	·2500	·2494	·2488	·2481	·2475	·2469	·2463	·2457	·2451	·2445	1	1	2	2	3	4	4	5	5
4·1	·2439	·2433	·2427	·2421	·2415	·2410	·2404	·2398	·2392	·2387	1	1	2	2	3	3	4	5	5
4·2	·2381	·2375	·2370	·2364	·2358	·2353	·2347	·2342	·2336	·2331	1	1	2	2	3	3	4	4	5
4·3	·2326	·2320	·2315	·2309	·2304	·2299	·2294	·2288	·2283	·2278	1	1	2	2	3	3	4	4	5
4·4	·2273	·2268	·2262	·2257	·2252	·2247	·2242	·2237	·2232	·2227	1	1	2	2	3	3	4	4	5
4·5	·2222	·2217	·2212	·2208	·2203	·2198	·2193	·2188	·2183	·2179	0	1	1	2	2	3	3	4	4
4·6	·2174	·2169	·2165	·2160	·2155	·2151	·2146	·2141	·2137	·2132	0	1	1	2	2	3	3	4	4
4·7	·2128	·2123	·2119	·2114	·2110	·2105	·2101	·2096	·2092	·2088	0	1	1	2	2	3	3	4	4
4·8	·2083	·2079	·2075	·2070	·2066	·2062	·2058	·2053	·2049	·2045	0	1	1	2	2	3	3	3	4
4·9	·2041	·2037	·2033	·2028	·2024	·2020	·2016	·2012	·2008	·2004	0	1	1	2	2	2	3	3	4
5·0	·2000	·1996	·1992	·1988	·1984	·1980	·1976	·1972	·1969	·1965	0	1	1	2	2	2	3	3	4
5·1	·1961	·1957	·1953	·1949	·1946	·1942	·1938	·1934	·1931	·1927	0	1	1	2	2	2	3	3	3
5·2	·1923	·1919	·1916	·1912	·1908	·1905	·1901	·1898	·1894	·1890	0	1	1	1	2	2	3	3	3
5·3	·1887	·1883	·1880	·1876	·1873	·1869	·1866	·1862	·1859	·1855	0	1	1	1	2	2	3	3	3
5·4	·1852	·1848	·1845	·1842	·1838	·1835	·1832	·1828	·1825	·1821	0	1	1	1	2	2	2	3	3
	0	1	2	3	4	5	6	7	8	9	1	2	3	4	5	6	7	8	9

RECIPROCALS

SUBTRACT

	0	1	2	3	4	5	6	7	8	9	1	2	3	4	5	6	7	8	9
5·5	·1818	·1815	·1812	·1808	·1805	·1802	·1799	·1795	·1792	·1789	0	1	1	1	2	2	2	3	3
5·6	·1786	·1783	·1779	·1776	·1773	·1770	·1767	·1764	·1761	·1757	0	1	1	1	2	2	2	3	3
5·7	·1754	·1751	·1748	·1745	·1742	·1739	·1736	·1733	·1730	·1727	0	1	1	1	2	2	2	2	3
5·8	·1724	·1721	·1718	·1715	·1712	·1709	·1706	·1704	·1701	·1698	0	1	1	1	1	2	2	2	3
5·9	·1695	·1692	·1689	·1686	·1684	·1681	·1678	·1675	·1672	·1669	0	1	1	1	1	2	2	2	3
6·0	·1667	·1664	·1661	·1658	·1656	·1653	·1650	·1647	·1645	·1642	0	1	1	1	1	2	2	2	3
6·1	·1639	·1637	·1634	·1631	·1629	·1626	·1623	·1621	·1618	·1616	0	1	1	1	1	2	2	2	2
6·2	·1613	·1610	·1608	·1605	·1603	·1600	·1597	·1595	·1592	·1590	0	1	1	1	1	2	2	2	2
6·3	·1587	·1585	·1582	·1580	·1577	·1575	·1572	·1570	·1567	·1565	0	0	1	1	1	1	2	2	2
6·4	·1563	·1560	·1558	·1555	·1553	·1550	·1548	·1546	·1543	·1541	0	0	1	1	1	1	2	2	2
6·5	·1538	·1536	·1534	·1531	·1529	·1527	·1524	·1522	·1520	·1517	0	0	1	1	1	1	2	2	2
6·6	·1515	·1513	·1511	·1508	·1506	·1504	·1502	·1499	·1497	·1495	0	0	1	1	1	1	2	2	2
6·7	·1493	·1490	·1488	·1486	·1484	·1481	·1479	·1477	·1475	·1473	0	0	1	1	1	1	2	2	2
6·8	·1471	·1468	·1466	·1464	·1462	·1460	·1458	·1456	·1453	·1451	0	0	1	1	1	1	2	2	2
6·9	·1449	·1447	·1445	·1443	·1441	·1439	·1437	·1435	·1433	·1431	0	0	1	1	1	1	1	2	2
7·0	·1429	·1427	·1425	·1422	·1420	·1418	·1416	·1414	·1412	·1410	0	0	1	1	1	1	1	2	2
7·1	·1408	·1406	·1404	·1403	·1401	·1399	·1397	·1395	·1393	·1391	0	0	1	1	1	1	1	2	2
7·2	·1389	·1387	·1385	·1383	·1381	·1379	·1377	·1376	·1374	·1372	0	0	1	1	1	1	1	2	2
7·3	·1370	·1368	·1366	·1364	·1362	·1361	·1359	·1357	·1355	·1353	0	0	1	1	1	1	1	2	2
7·4	·1351	·1350	·1348	·1346	·1344	·1342	·1340	·1339	·1337	·1335	0	0	1	1	1	1	1	1	2
7·5	·1333	·1332	·1330	·1328	·1326	·1325	·1323	·1321	·1319	·1318	0	0	1	1	1	1	1	1	2
7·6	·1316	·1314	·1312	·1311	·1309	·1307	·1305	·1304	·1302	·1300	0	0	1	1	1	1	1	1	2
7·7	·1299	·1297	·1295	·1294	·1292	·1290	·1289	·1287	·1285	·1284	0	0	0	1	1	1	1	1	1
7·8	·1282	·1280	·1279	·1277	·1276	·1274	·1272	·1271	·1269	·1267	0	0	0	1	1	1	1	1	1
7·9	·1266	·1264	·1263	·1261	·1259	·1258	·1256	·1255	·1253	·1252	0	0	0	1	1	1	1	1	1
8·0	·1250	·1248	·1247	·1245	·1244	·1242	·1241	·1239	·1238	·1236	0	0	0	1	1	1	1	1	1
8·1	·1235	·1233	·1232	·1230	·1229	·1227	·1225	·1224	·1222	·1221	0	0	0	1	1	1	1	1	1
8·2	·1220	·1218	·1217	·1215	·1214	·1212	·1211	·1209	·1208	·1206	0	0	0	1	1	1	1	1	1
8·3	·1205	·1203	·1202	·1200	·1199	·1198	·1196	·1195	·1193	·1192	0	0	0	1	1	1	1	1	1
8·4	·1190	·1189	·1188	·1186	·1185	·1183	·1182	·1181	·1179	·1178	0	0	0	1	1	1	1	1	1
8·5	·1176	·1175	·1174	·1172	·1171	·1170	·1168	·1167	·1166	·1164	0	0	0	1	1	1	1	1	1
8·6	·1163	·1161	·1160	·1159	·1157	·1156	·1155	·1153	·1152	·1151	0	0	0	1	1	1	1	1	1
8·7	·1149	·1148	·1147	·1145	·1144	·1143	·1142	·1140	·1139	·1138	0	0	0	1	1	1	1	1	1
8·8	·1136	·1135	·1134	·1133	·1131	·1130	·1129	·1127	·1126	·1125	0	0	0	1	1	1	1	1	1
8·9	·1124	·1122	·1121	·1120	·1119	·1117	·1116	·1115	·1114	·1112	0	0	0	1	1	1	1	1	1
9·0	·1111	·1110	·1109	·1107	·1106	·1105	·1104	·1103	·1101	·1100	0	0	0	1	1	1	1	1	1
9·1	·1099	·1098	·1096	·1095	·1094	·1093	·1092	·1091	·1089	·1088	0	0	0	0	1	1	1	1	1
9·2	·1087	·1086	·1085	·1083	·1082	·1081	·1080	·1079	·1078	·1076	0	0	0	0	1	1	1	1	1
9·3	·1075	·1074	·1073	·1072	·1071	·1070	·1068	·1067	·1066	·1065	0	0	0	0	1	1	1	1	1
9·4	·1064	·1063	·1062	·1060	·1059	·1058	·1057	·1056	·1055	·1054	0	0	0	0	1	1	1	1	1
9·5	·1053	·1052	·1050	·1049	·1048	·1047	·1046	·1045	·1044	·1043	0	0	0	0	1	1	1	1	1
9·6	·1042	·1041	·1040	·1038	·1037	·1036	·1035	·1034	·1033	·1032	0	0	0	0	1	1	1	1	1
9·7	·1031	·1030	·1029	·1028	·1027	·1026	·1025	·1024	·1022	·1021	0	0	0	0	1	1	1	1	1
9·8	·1020	·1019	·1018	·1017	·1016	·1015	·1014	·1013	·1012	·1011	0	0	0	0	1	1	1	1	1
9·9	·1010	·1009	·1008	·1007	·1006	·1005	·1004	·1003	·1002	·1001	0	0	0	0	0	1	1	1	1
	0	1	2	3	4	5	6	7	8	9	1	2	3	4	5	6	7	8	9

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