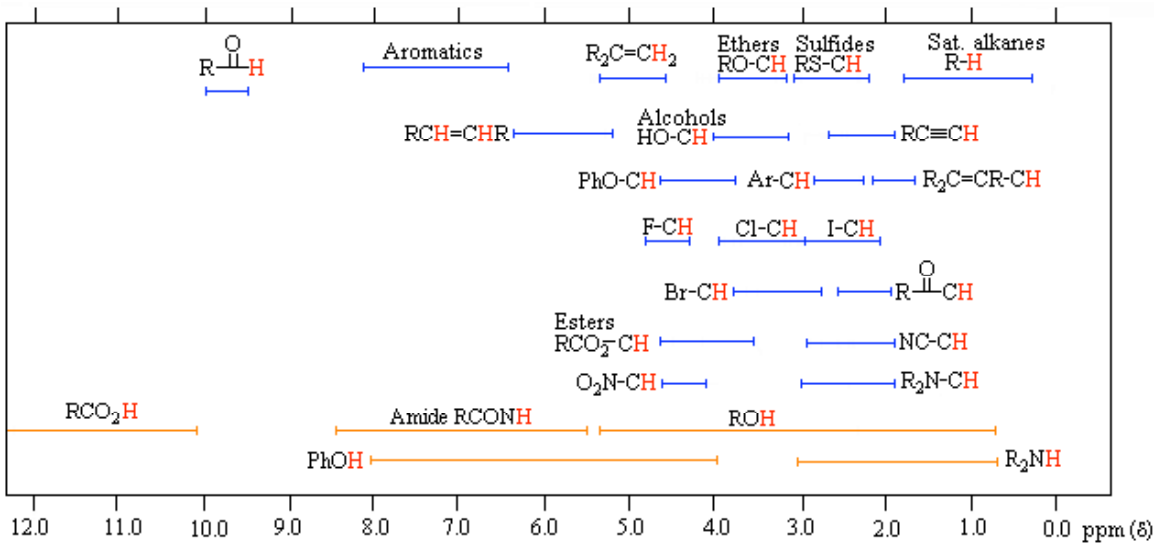
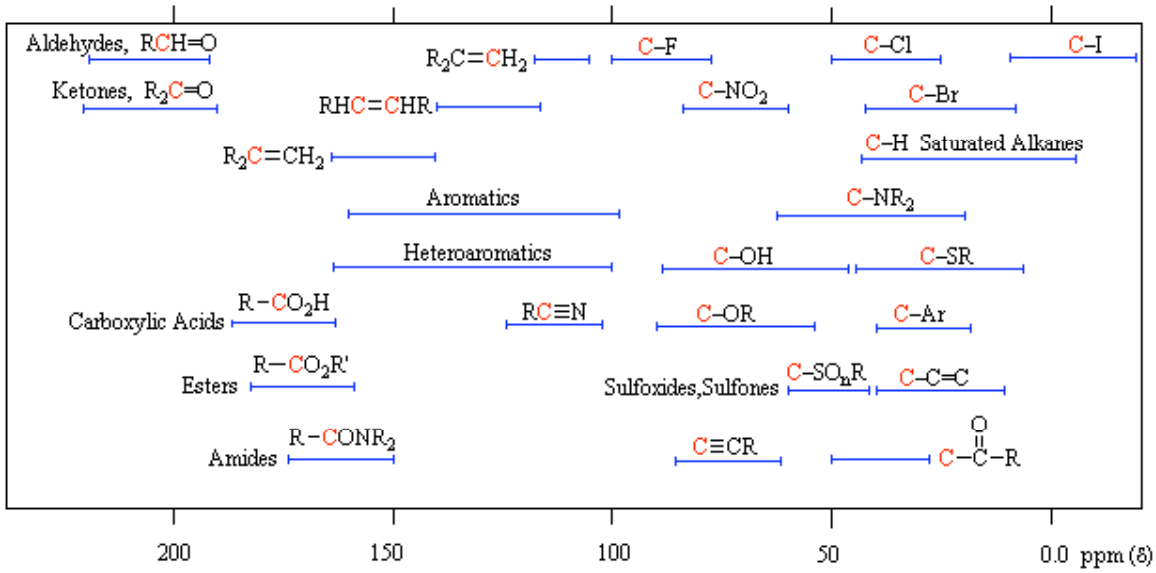
^{1}H chemical shift ranges

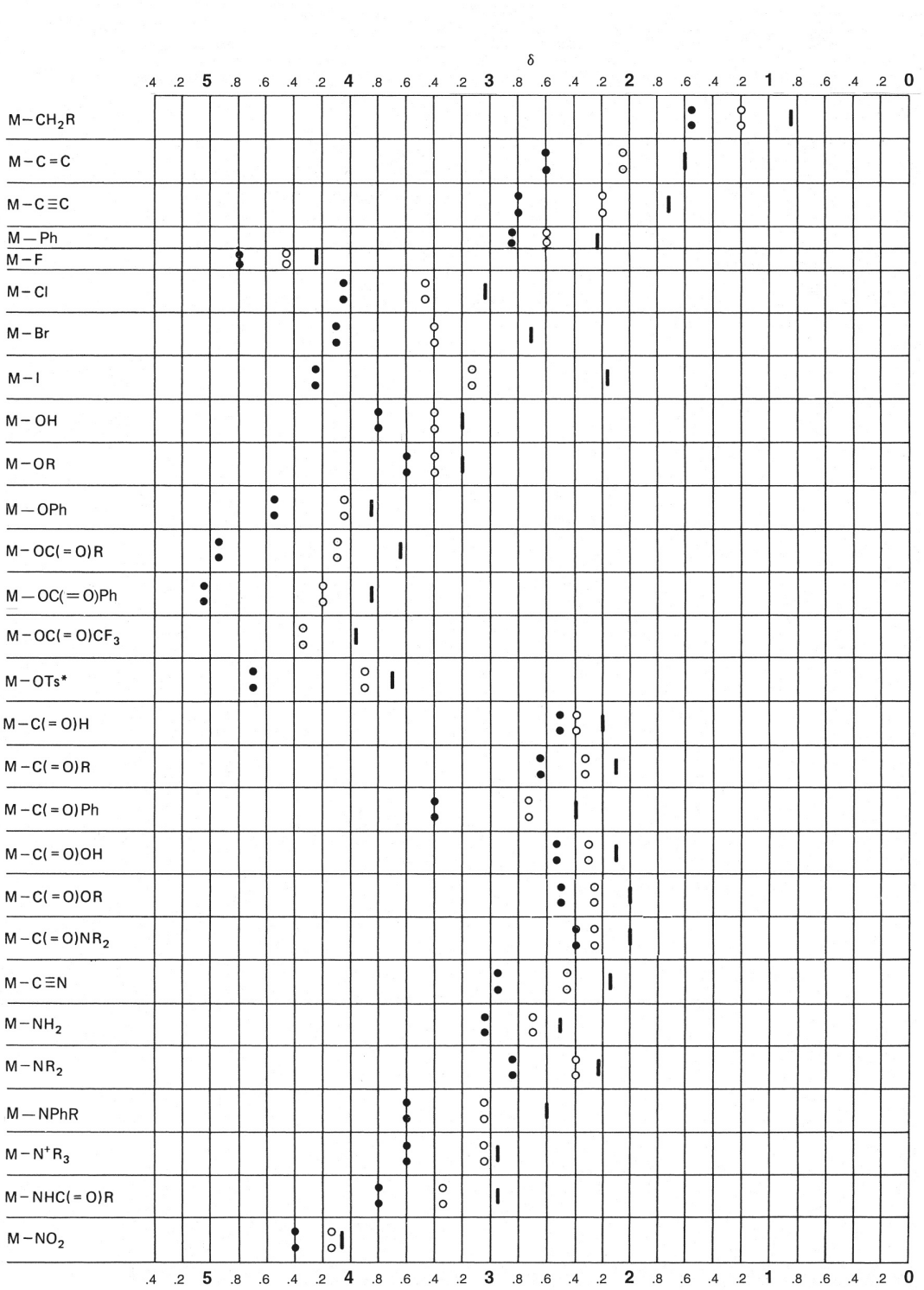


^{13}C chemical shift ranges



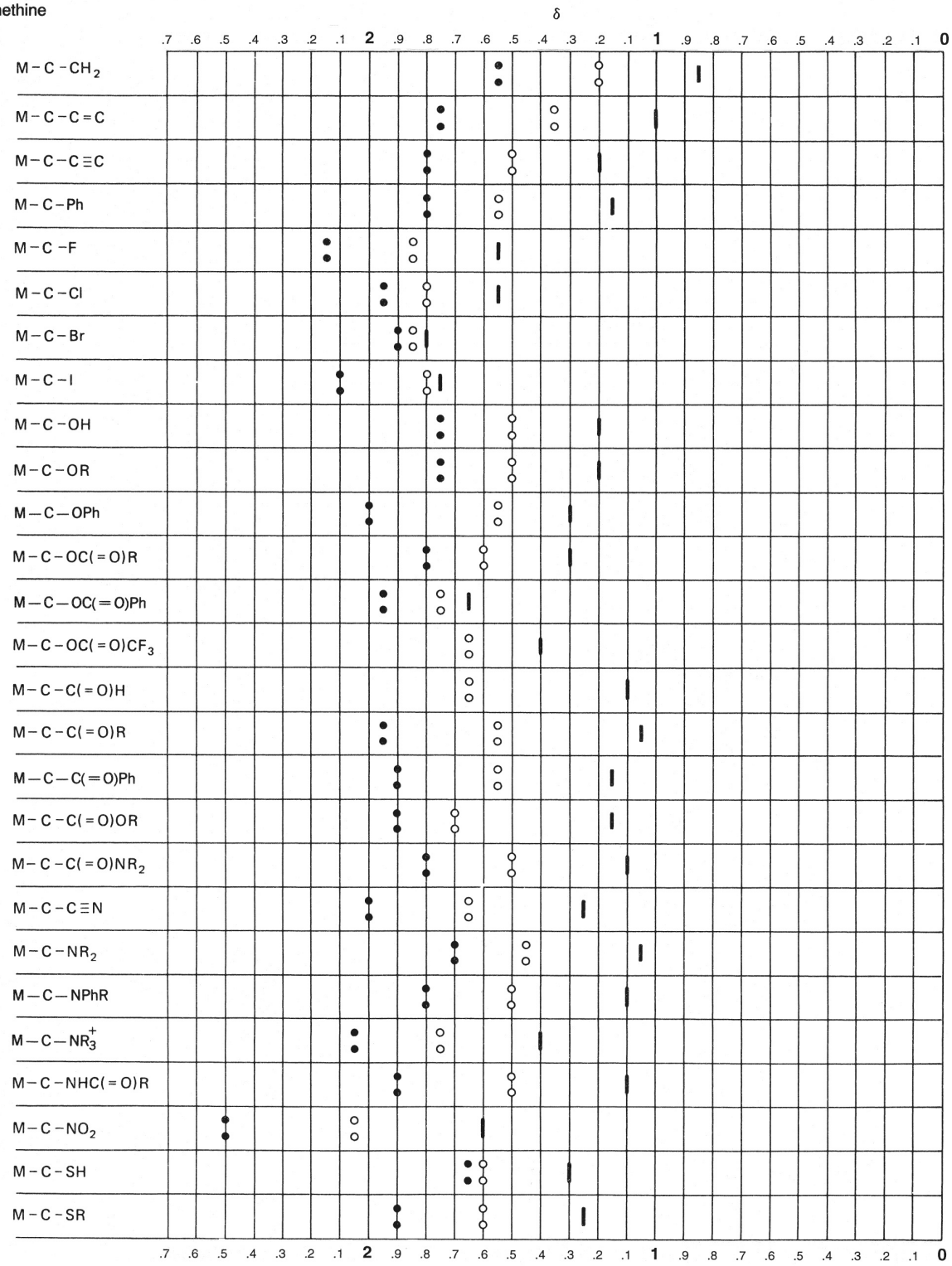
APPENDIX A

CHART A.1 CHEMICAL SHIFTS OF PROTONS ON A CARBON ATOM ADJACENT (α POSITION) TO A FUNCTIONAL GROUP IN ALIPHATIC COMPOUNDS (M—Y)

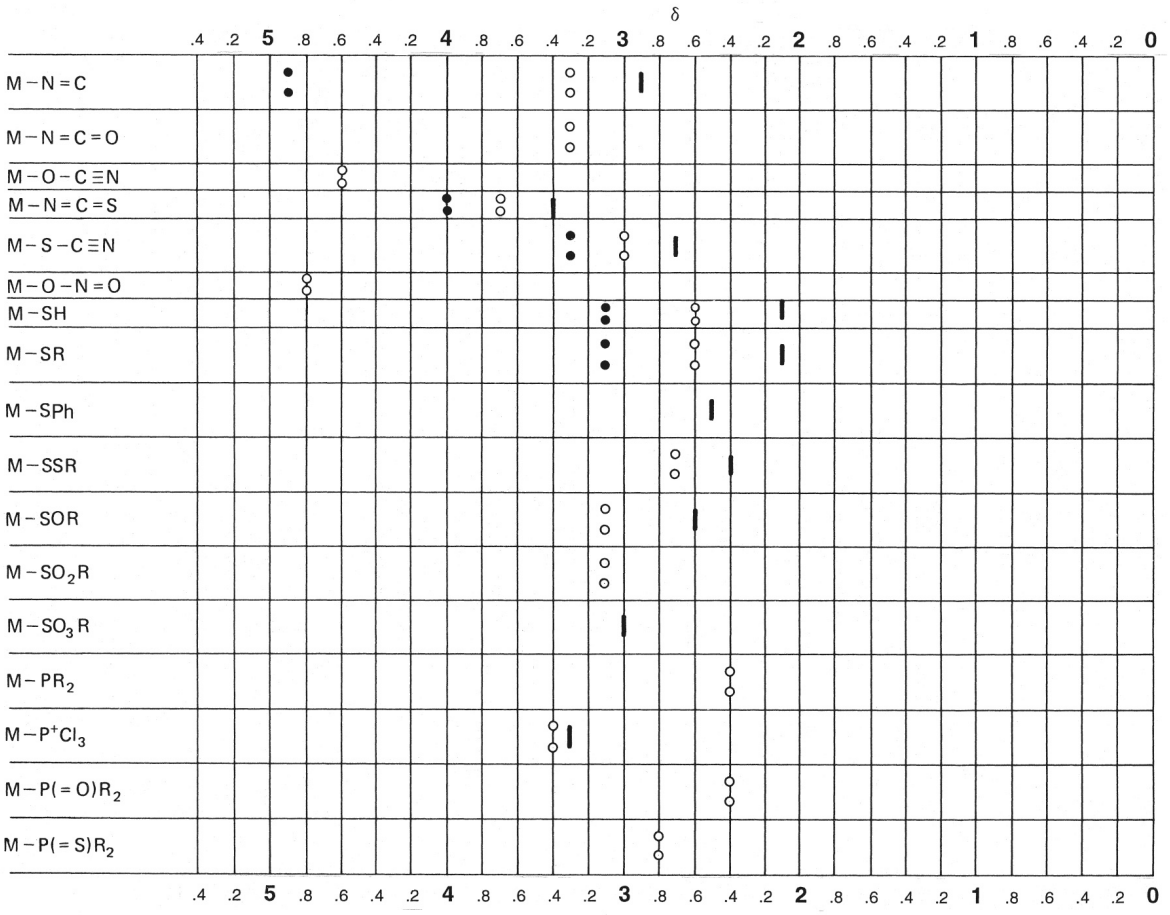


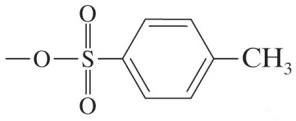
APPENDIX A CHART A.2 CHEMICAL SHIFTS OF PROTONS ON A CARBON ATOM ONCE REMOVED (β POSITION) FROM A FUNCTIONAL GROUP IN ALIPHATIC COMPOUNDS (M—C—Y)

▮ M = methyl
8 M = methylene
⁝ M = methine



APPENDIX A *(Continued)*



*OTS is 

APPENDIX C THE ^{13}C CORRELATION CHART FOR CHEMICAL CLASSES

R = H or alkyl subsituents
Y = polar substituents

Acyclic hydrocarbons

$-CH_3$

$-CH_2-$

$-CH<$

$-C(<)_2$

Alicyclic hydrocarbons

C_3H_6

C_4H_8 to $C_{10}H_{20}$

Alkenes

$H_2C=C-R$

$H_2C=C-Y$

$C=C-C=C-R$

Allenes

$C=C=C$

Alkynes

$C\equiv C-R$

$C\equiv C-Y$

Aromatics

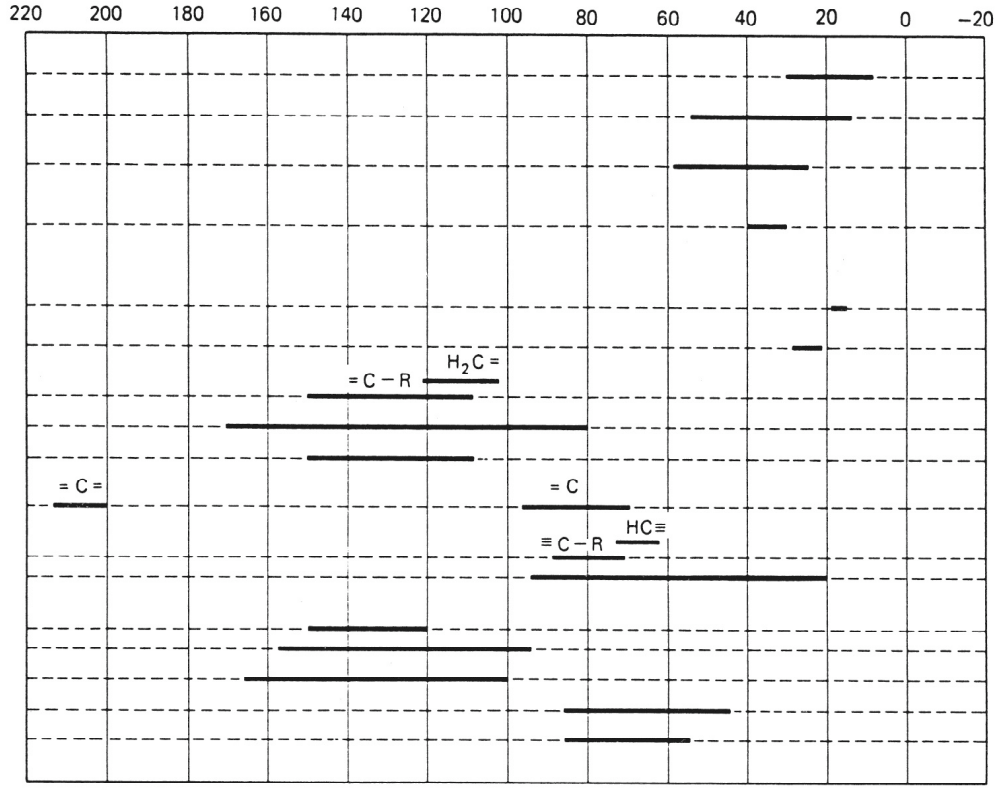
$Ar-R$

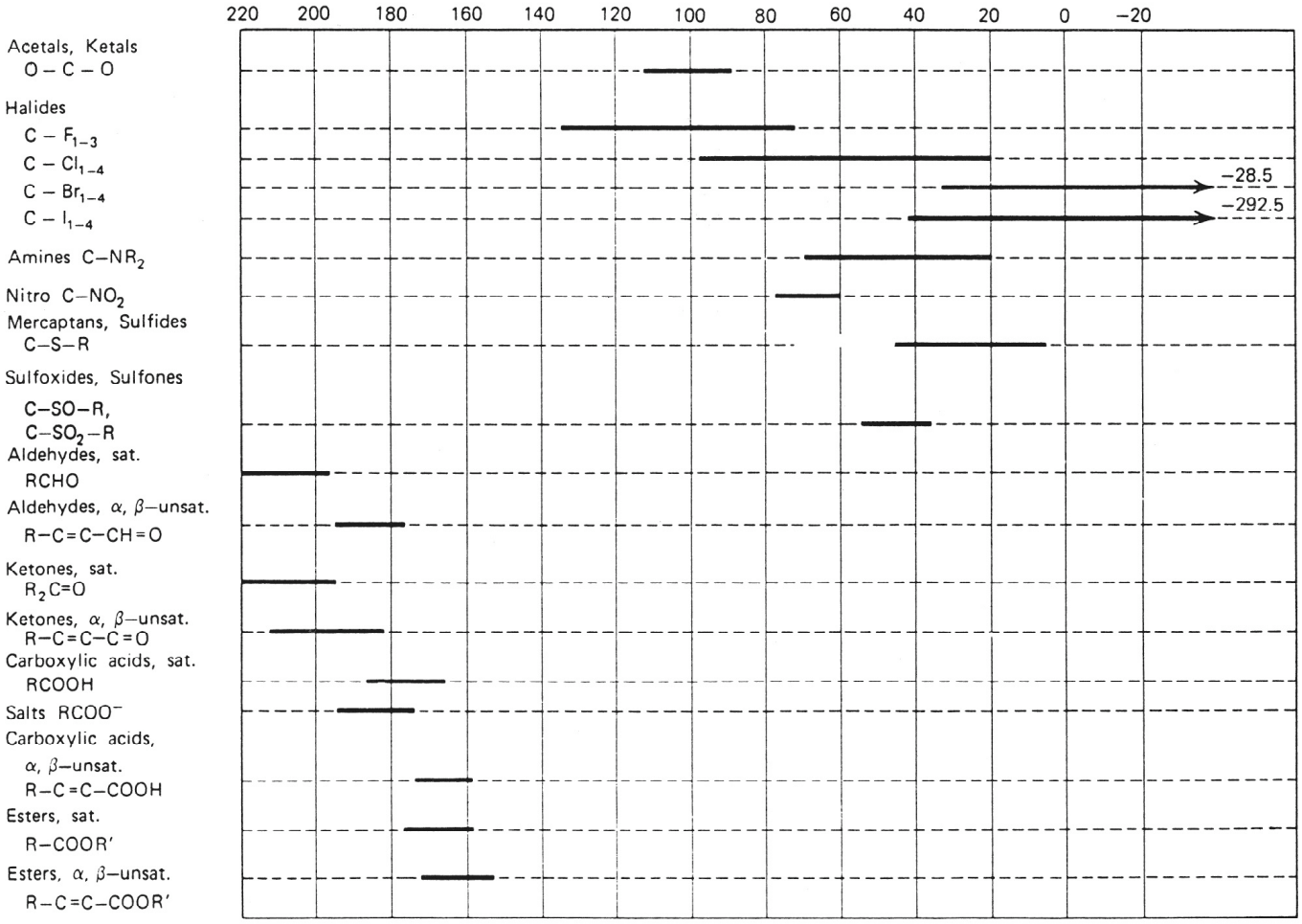
$Ar-Y$

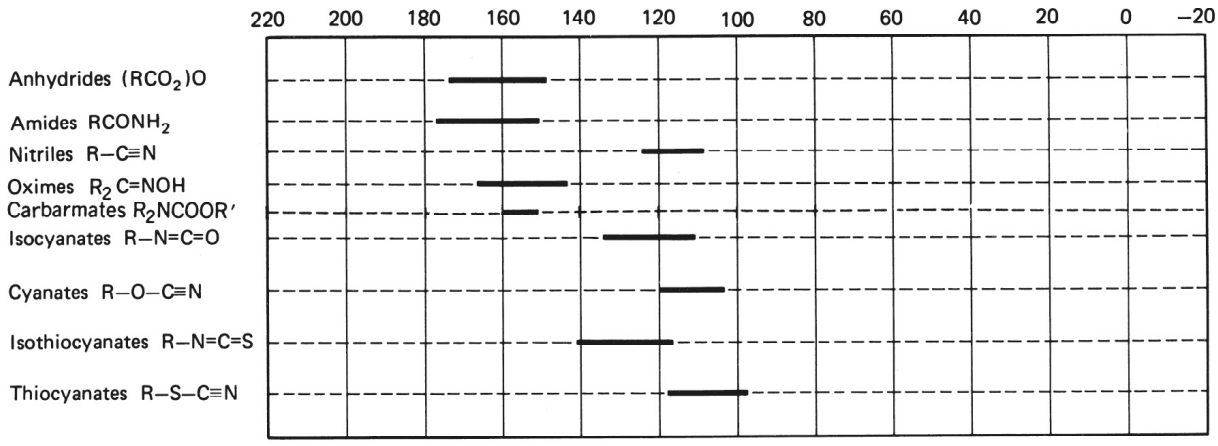
Heteroaromatics

Alcohols C–OH

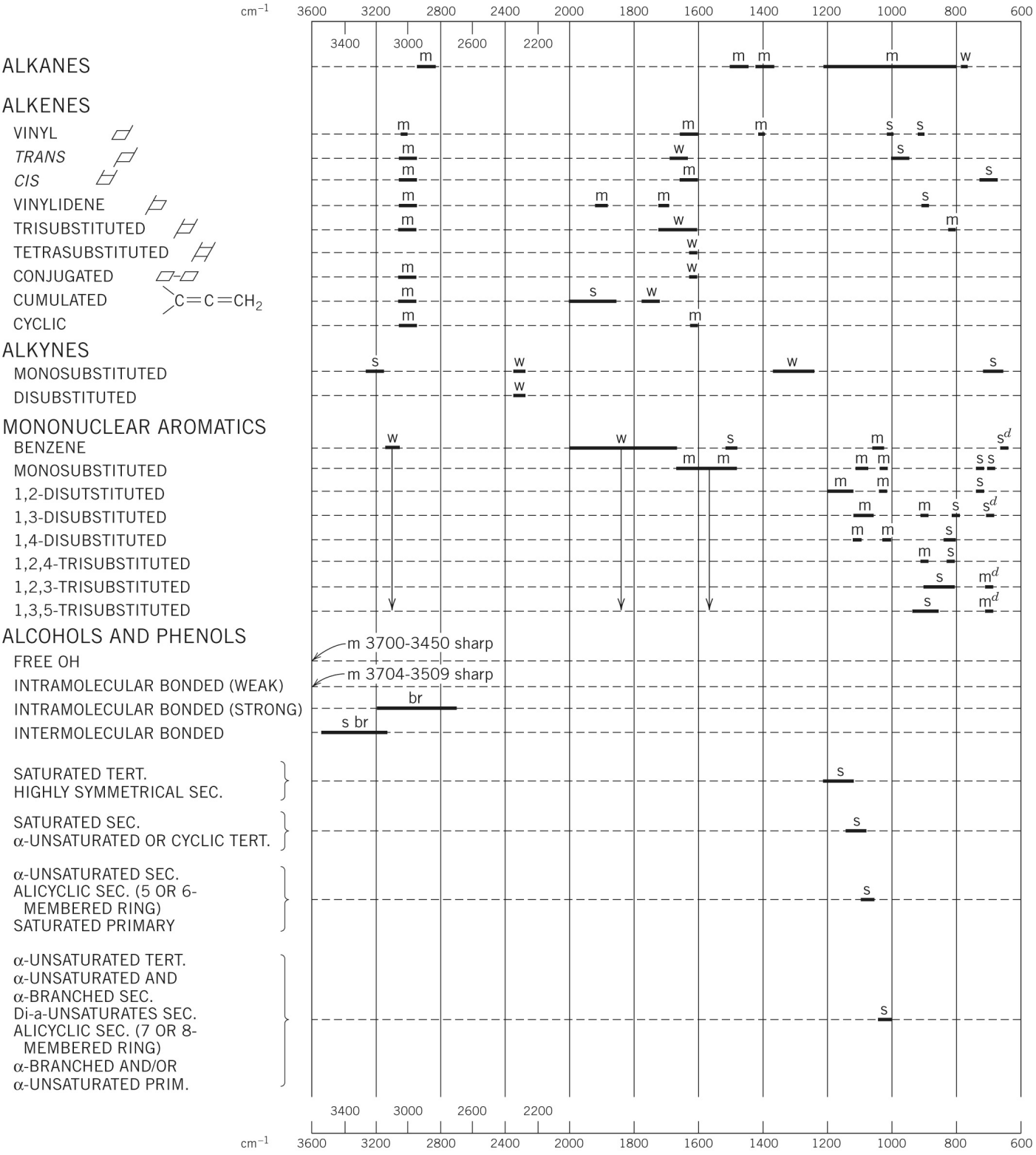
Ethers C–O–C




220 200 180 160 140 120 100 80 60 40 20 0 −20
Acetals, Ketals
O − C − O
Halides
C − F1−3
C − Cl1−4
C − Br1−4
C − I1−4
Amines C−NR2
Nitro C−NO2
Mercaptans, Sulfides
C−S−R
Sulfoxides, Sulfones
C−SO−R,
C−SO2−R
Aldehydes, sat.
RCHO
Aldehydes, α, β−unsat.
R−C=C−CH=O
Ketones, sat.
R2C=O
Ketones, α, β−unsat.
R−C=C−C=O
Carboxylic acids, sat.
RCOOH
Salts RCOO−
Carboxylic acids,
α, β−unsat.
R−C=C−COOH
Esters, sat.
R−COOR′
Esters, α, β−unsat.
R−C=C−COOR′
−28.5
−292.5


220 200 180 160 140 120 100 80 60 40 20 0 −20
Anhydrides (RCO2)O
Amides RCONH2
Nitriles R−C≡N
Oximes R2C=NOH
Carbarmates R2NCOOR′
Isocyanates R−N=C=O
Cyanates R−O−C≡N
Isothiocyanates R−N=C=S
Thiocyanates R−S−C≡N

APPENDIX B CHARACTERISTIC GROUP ABSORPTIONS[a]

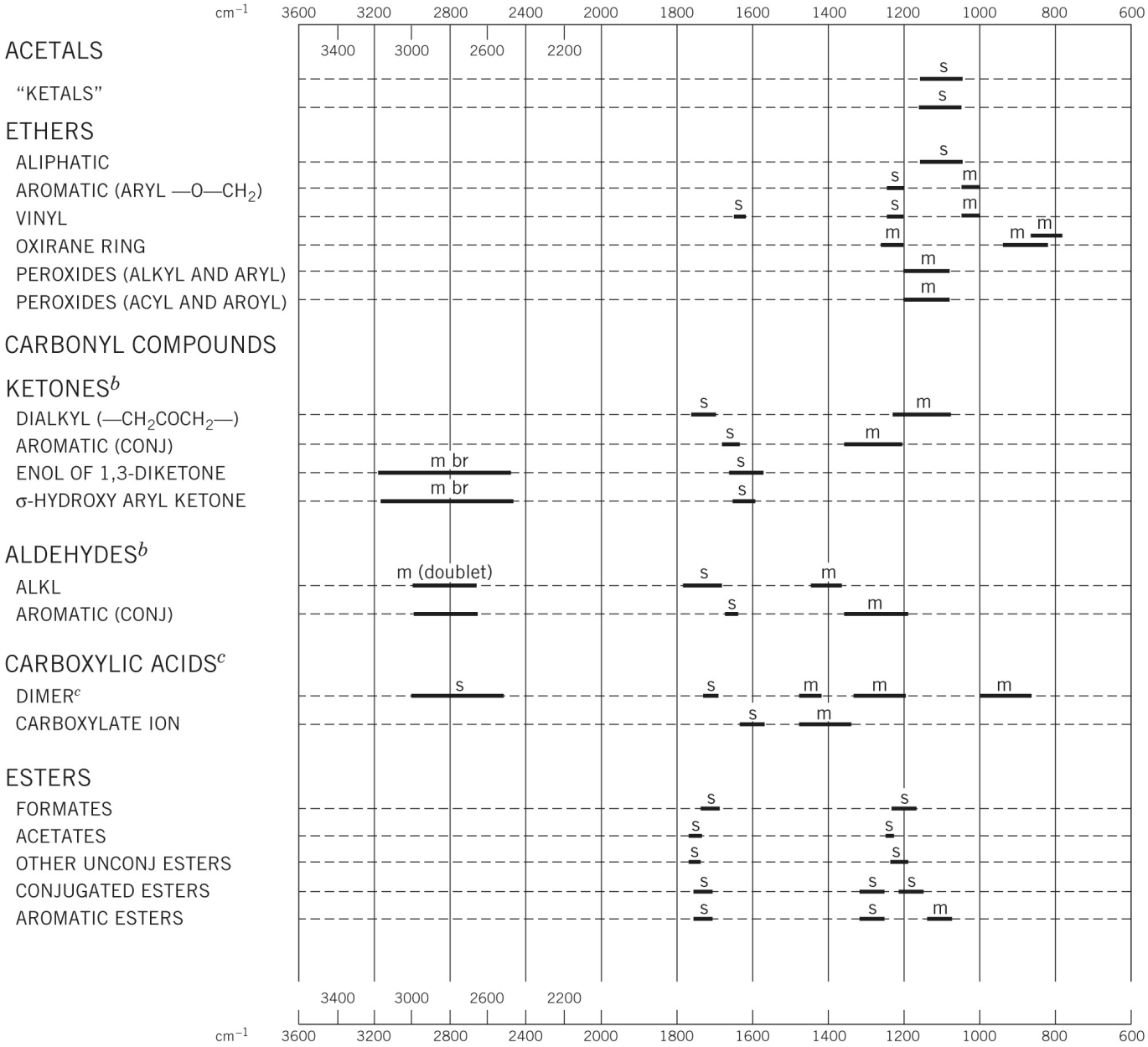


[a] Absorptions are shown by heavy bars. s = strong, m = medium, w = weak, sh = sharp, br = broad. Two intensity designations over a single bar indicate that two peaks may be present.

[b] May be absent.

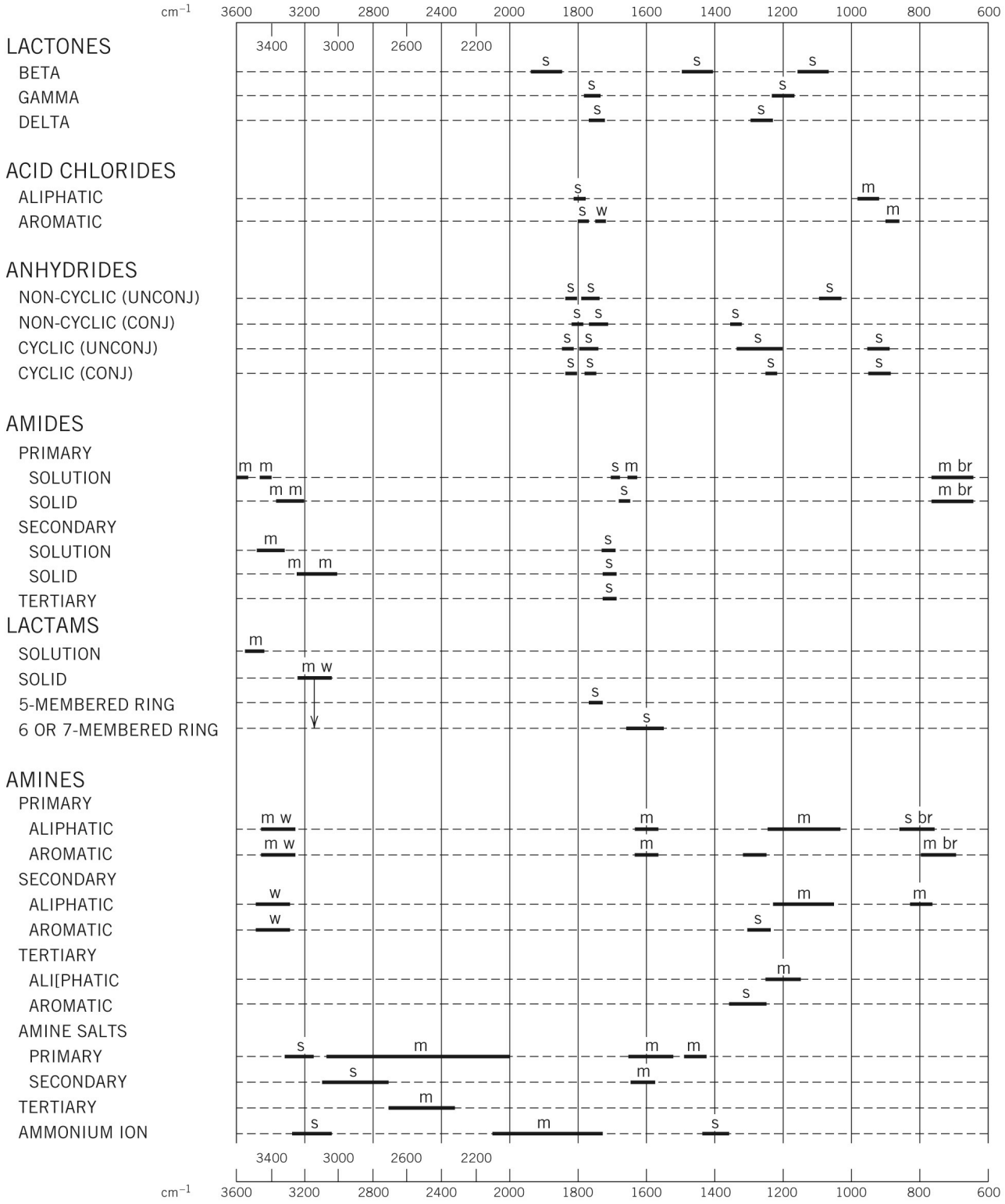
[c] Frequently a doublet.

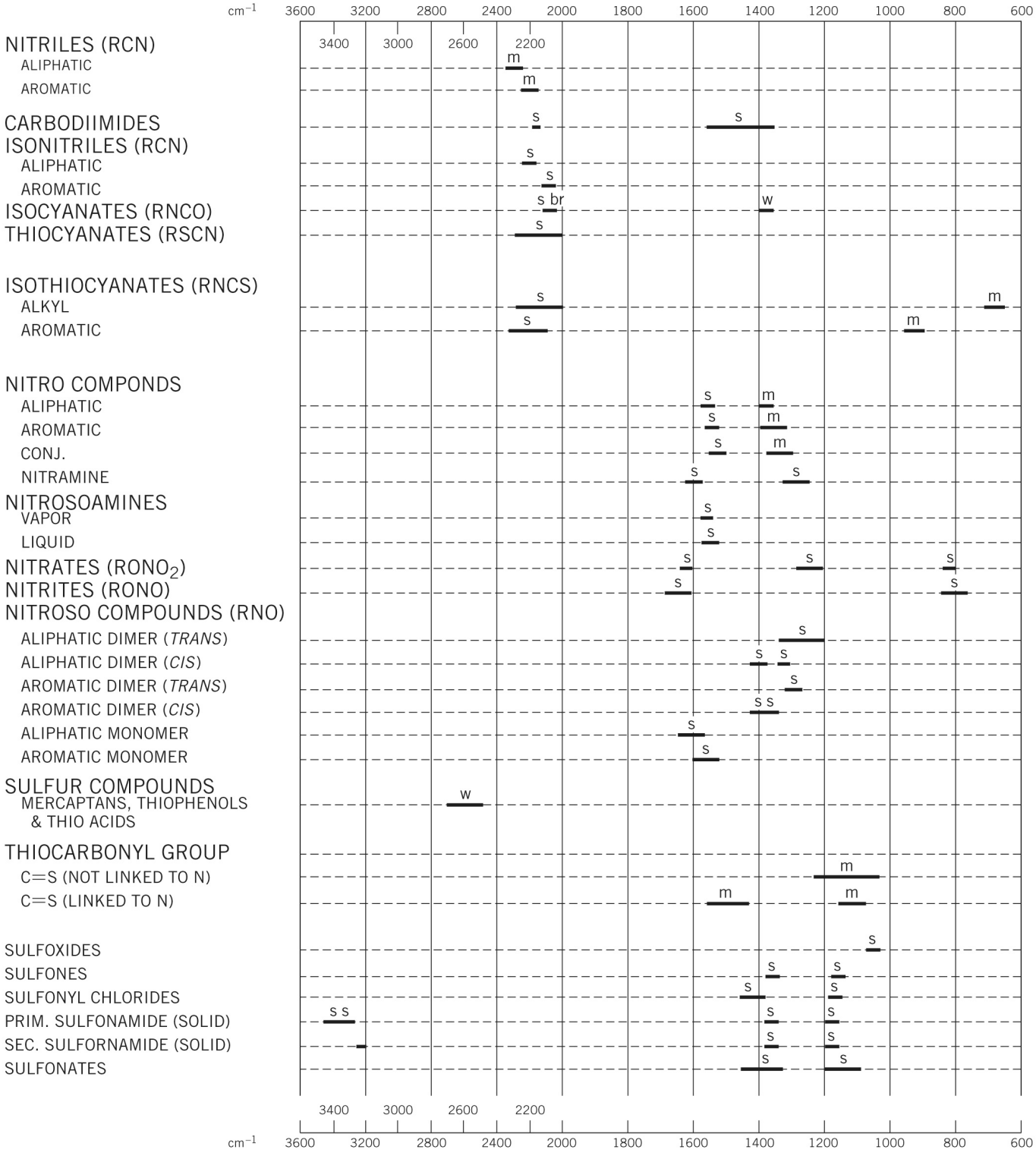
[d] Ring bending bands.



[a] Three bands, sometimes a fourth for ketals, and a fifth band for acetals.
[b] Conjugated aliphatic examples show C═O stretch at virtually the same position as aromatic structures.
[c] Conjugated examples show C═O stretch at lower wavenumbers (1710–1680 cm^{-1}). The O—H stretch (3300–2600 cm^{-1}) is very broad.

APPENDIX B *(Continued)*




cm⁻¹
3600 3200 2800 2400 2000 1800 1600 1400 1200 1000 800 600
3400 3000 2600 2200
NITRILES (RCN)
ALIPHATIC
AROMATIC
CARBODIIMIDES
ISONITRILES (RCN)
ALIPHATIC
AROMATIC
ISOCYANATES (RNCO)
THIOCYANATES (RSCN)
ISOTHIOCYANATES (RNCS)
ALKYL
AROMATIC
NITRO COMPONDS
ALIPHATIC
AROMATIC
CONJ.
NITRAMINE
NITROSOAMINES
VAPOR
LIQUID
NITRATES (RONO2)
NITRITES (RONO)
NITROSO COMPOUNDS (RNO)
ALIPHATIC DIMER (TRANS)
ALIPHATIC DIMER (CIS)
AROMATIC DIMER (TRANS)
AROMATIC DIMER (CIS)
ALIPHATIC MONOMER
AROMATIC MONOMER
SULFUR COMPOUNDS
MERCAPTANS, THIOPHENOLS & THIO ACIDS
THIOCARBONYL GROUP
C=S (NOT LINKED TO N)
C=S (LINKED TO N)
SULFOXIDES
SULFONES
SULFONYL CHLORIDES
PRIM. SULFONAMIDE (SOLID)
SEC. SULFORNAMIDE (SOLID)
SULFONATES

APPENDIX B *(Continued)*