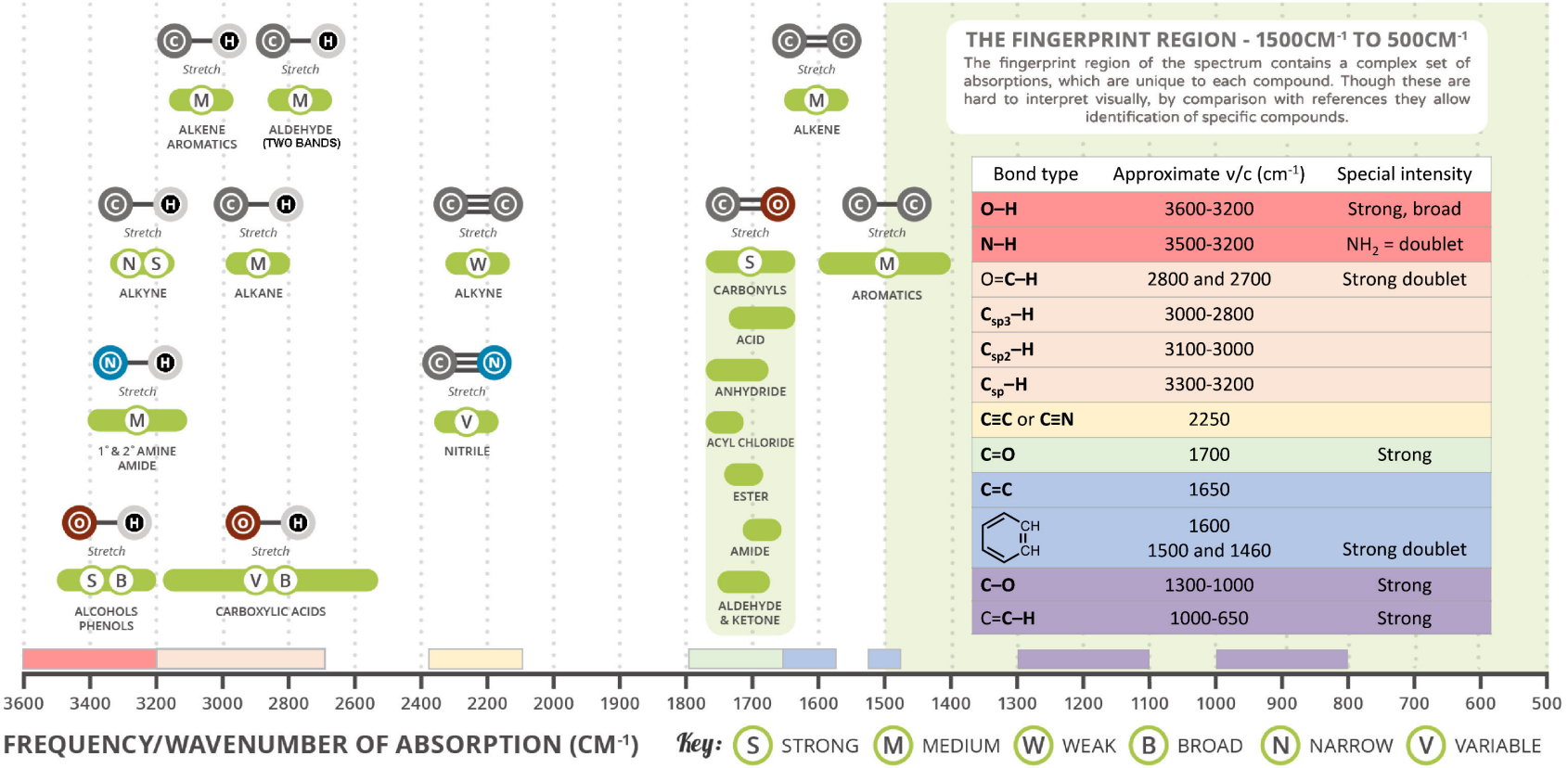
ANALYTICAL CHEMISTRY - INFRARED SPECTROSCOPY

Commonly referred to as IR spectroscopy, this technique allows chemists to identify characteristic groups of atoms (functional groups) present in molecules.



THE FINGERPRINT REGION - 1500CM^{-1} TO 500CM^{-1}

The fingerprint region of the spectrum contains a complex set of absorptions, which are unique to each compound. Though these are hard to interpret visually, by comparison with references they allow identification of specific compounds.

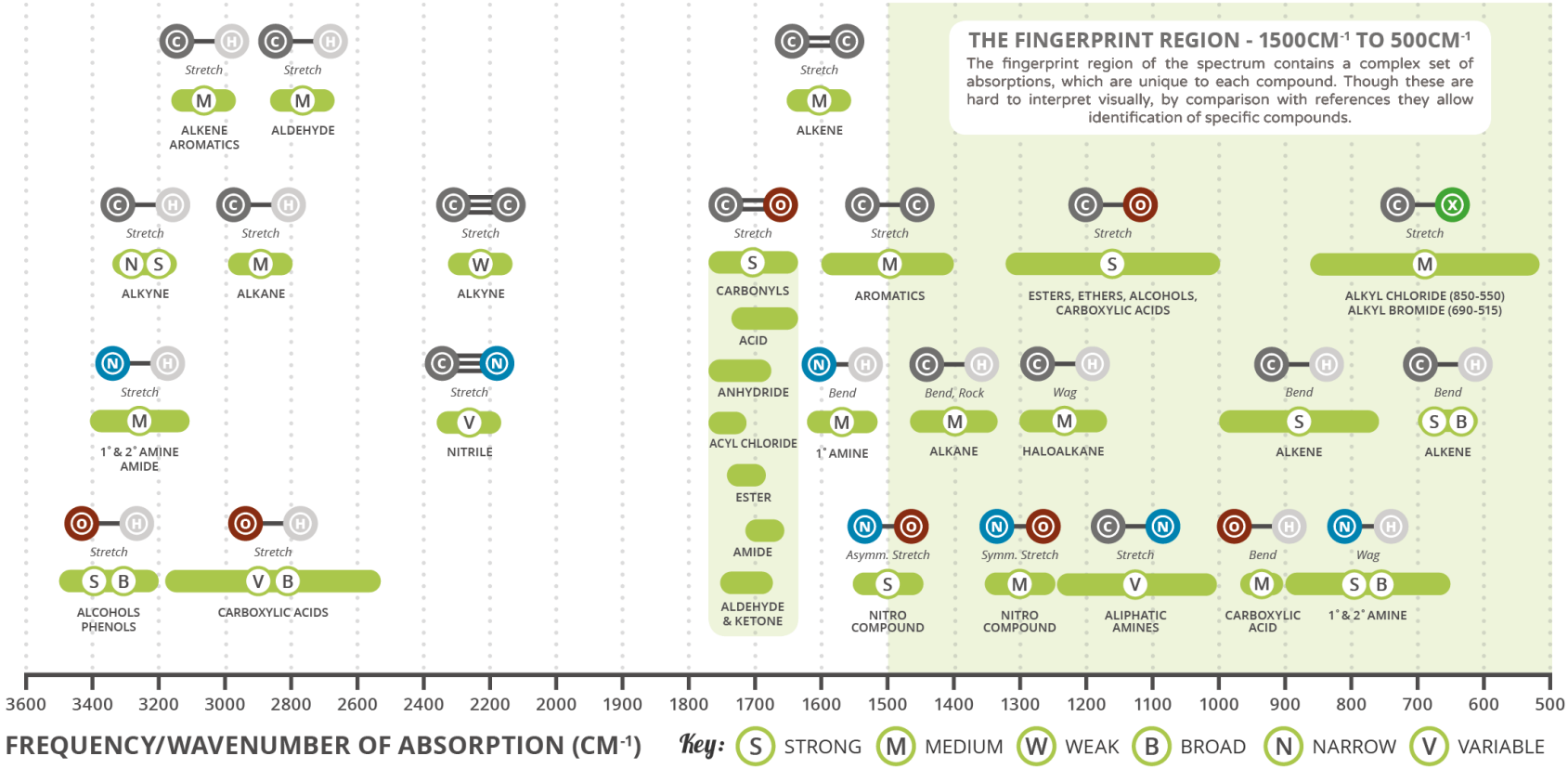
Bond type	Approximate ν/c (cm^{-1})	Special intensity
O–H	3600-3200	Strong, broad
N–H	3500-3200	NH_2 = doublet
O=**C–H**	2800 and 2700	Strong doublet
C_{sp3}–H	3000-2800	
C_{sp2}–H	3100-3000	
C_{sp}–H	3300-3200	
C≡C or **C≡N**	2250	
C=O	1700	Strong
C=C	1650	
	1600 1500 and 1460	Strong doublet
C–O	1300-1000	Strong
C=**C–H**	1000-650	Strong

Infrared frequencies make up a portion of the electromagnetic spectrum. If a range of infrared frequencies are shone through an organic compound, some of the frequencies are absorbed by the chemical bonds within the compound. Different chemical bonds absorb different frequencies of infrared radiation. There are a number of characteristic absorptions which allow functional groups (the parts of a compound which give it its particular reactivity) to be identified. This graphic shows a number of these absorptions.

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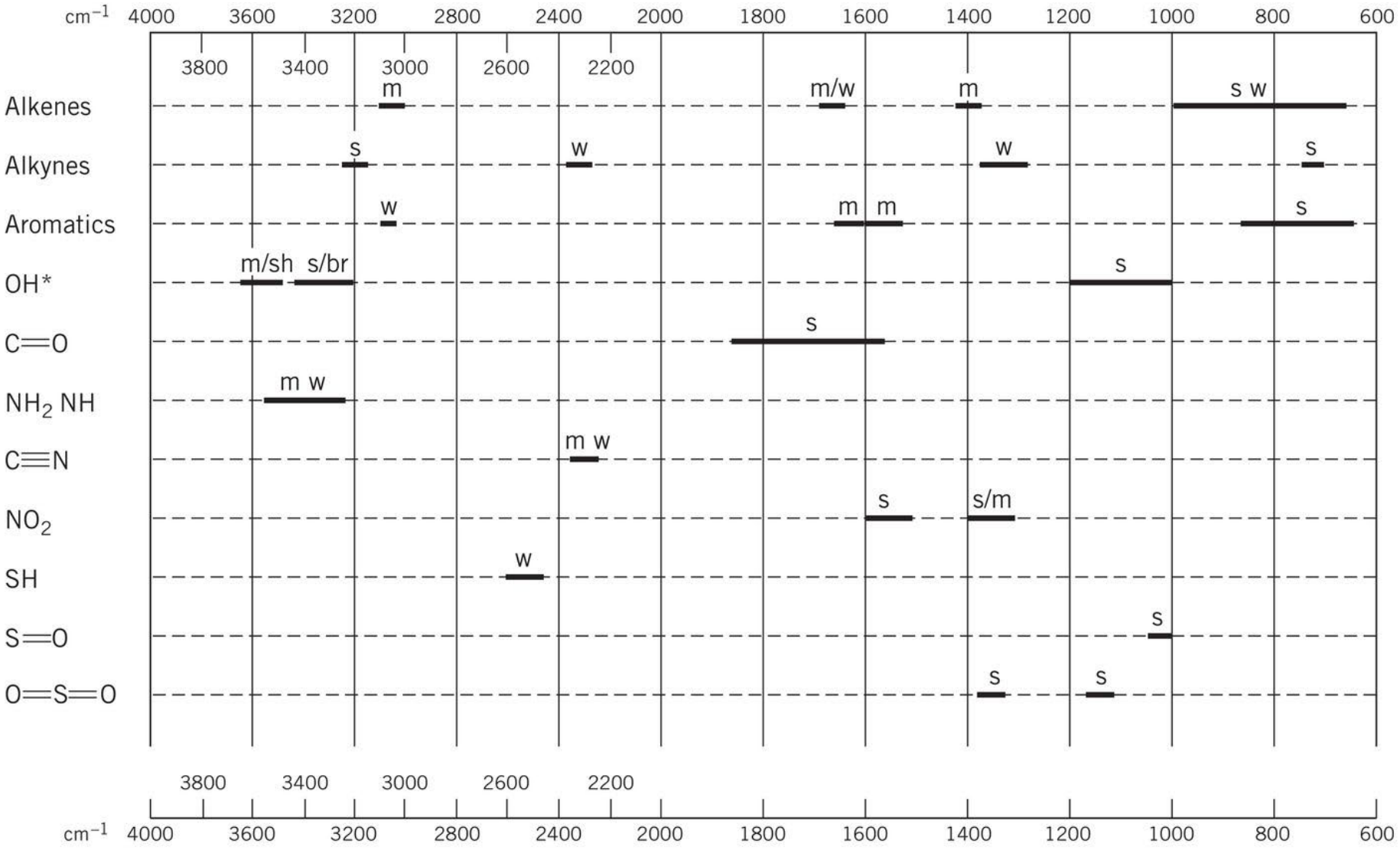
ANALYTICAL CHEMISTRY - INFRARED SPECTROSCOPY

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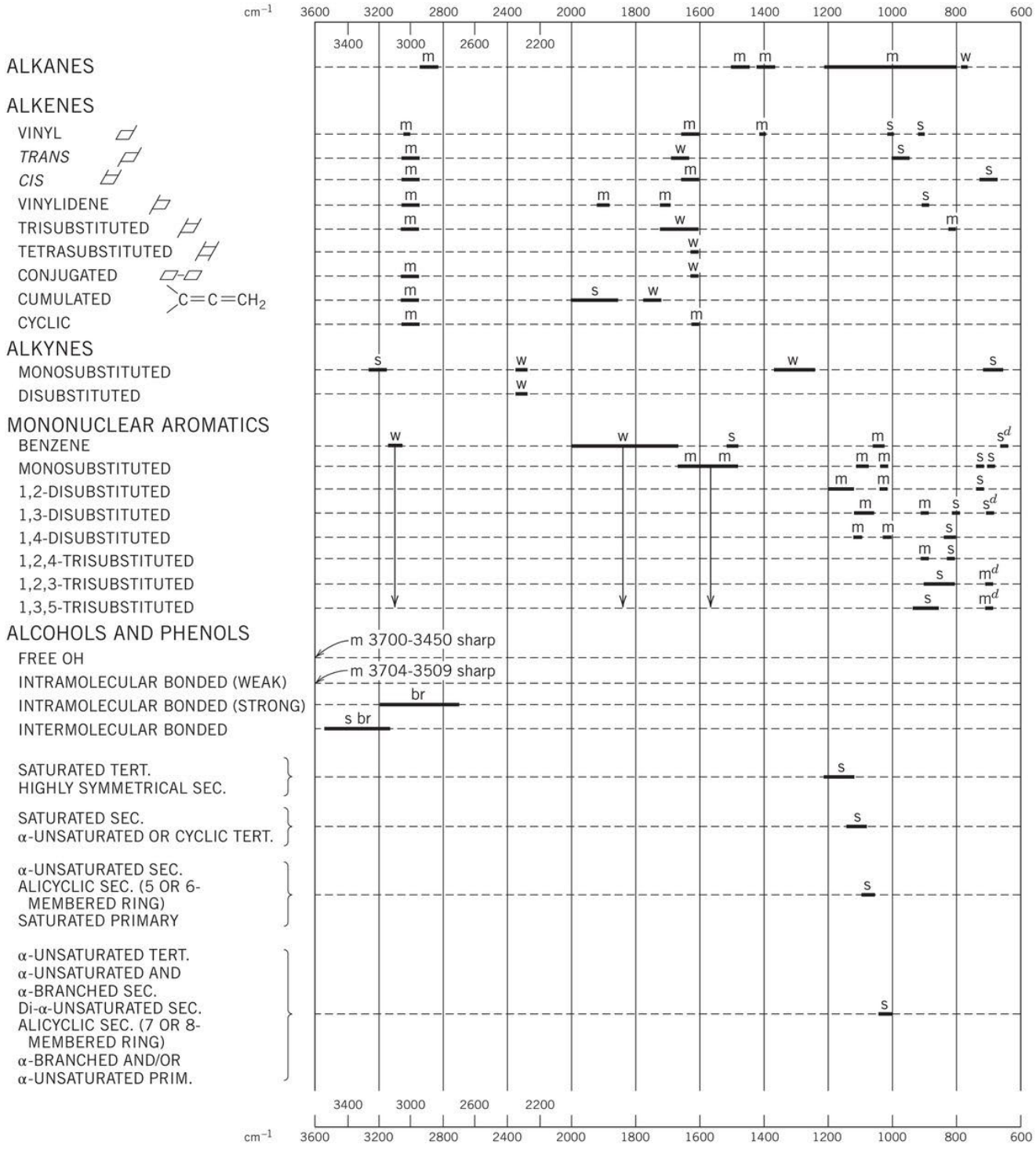


Infrared frequencies make up a portion of the electromagnetic spectrum. If a range of infrared frequencies are shone through an organic compound, some of the frequencies are absorbed by the chemical bonds within the compound. Different chemical bonds absorb different frequencies of infrared radiation. There are a number of characteristic absorptions which allow functional groups (the parts of a compound which give it its particular reactivity) to be identified. This graphic shows a number of these absorptions.

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*Free OH, medium and sharp; bonded OH, strong and broad

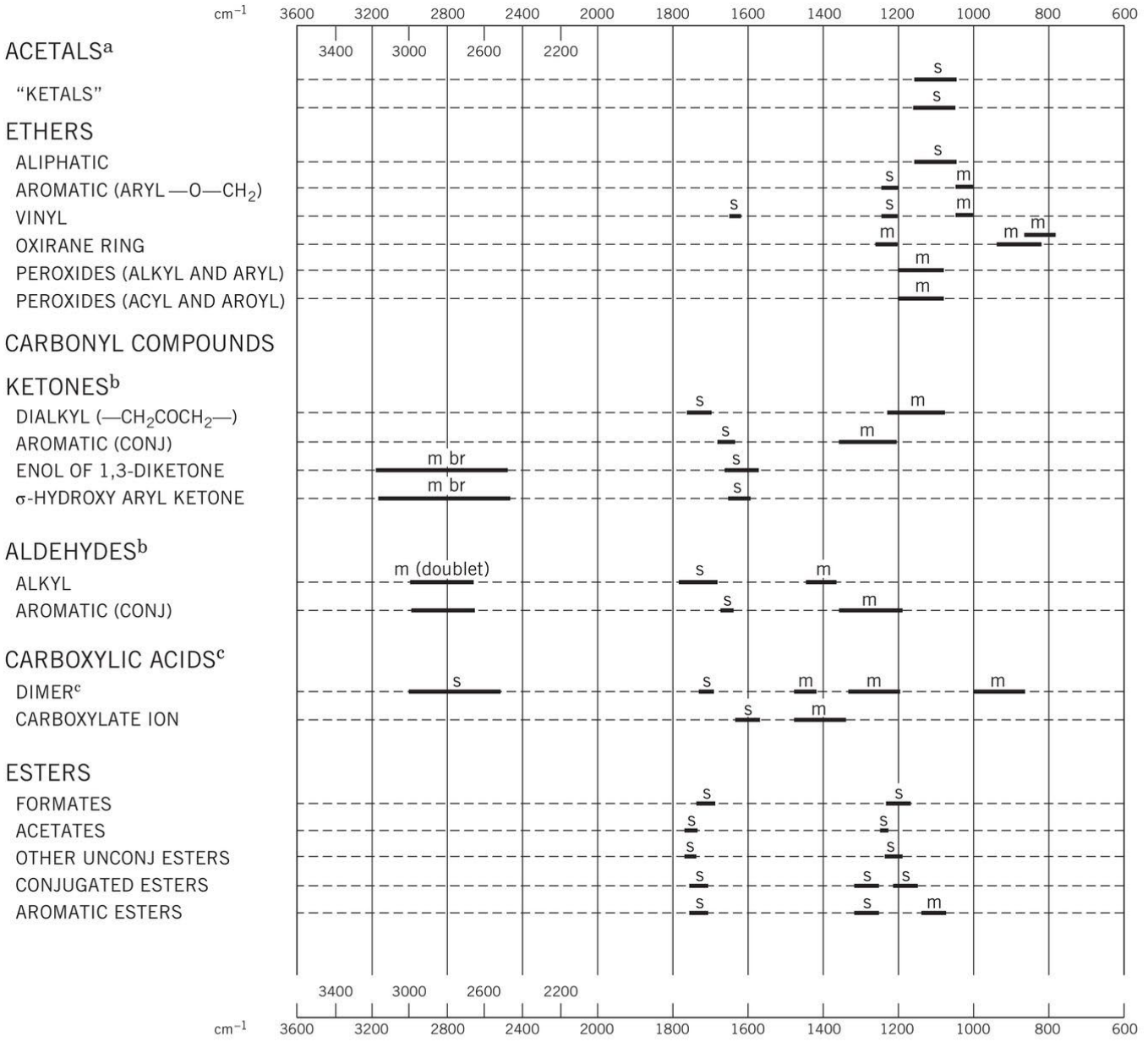


[a] Absorptions are shown by heavy bars. s = strong, m = medium, w = weak, sh = sharp, br = broad. Two intensity designations over a single bar indicate that two peaks may be present.

[b] May be absent.

[c] Frequently a doublet.

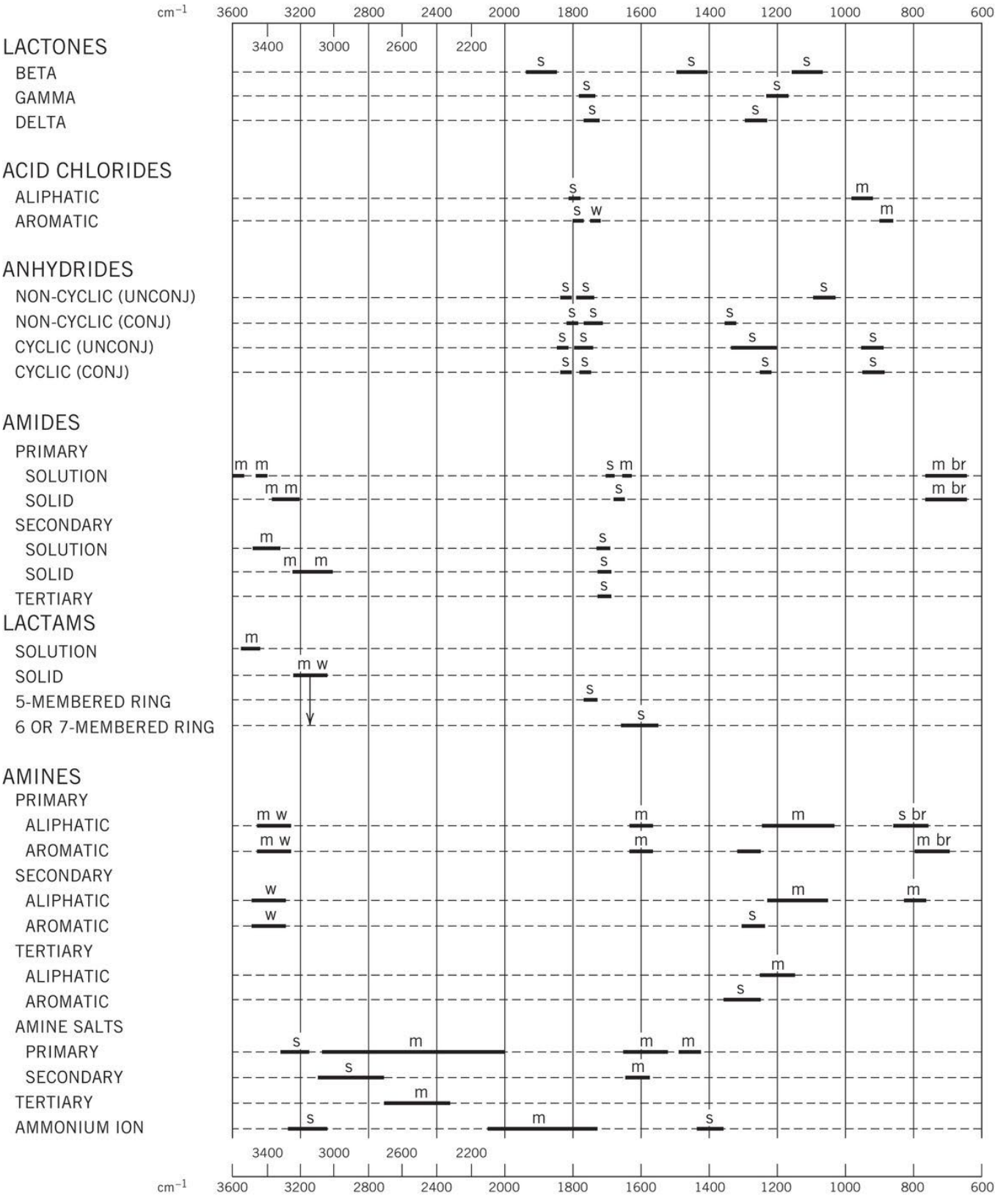
[d] Ring bending bands.

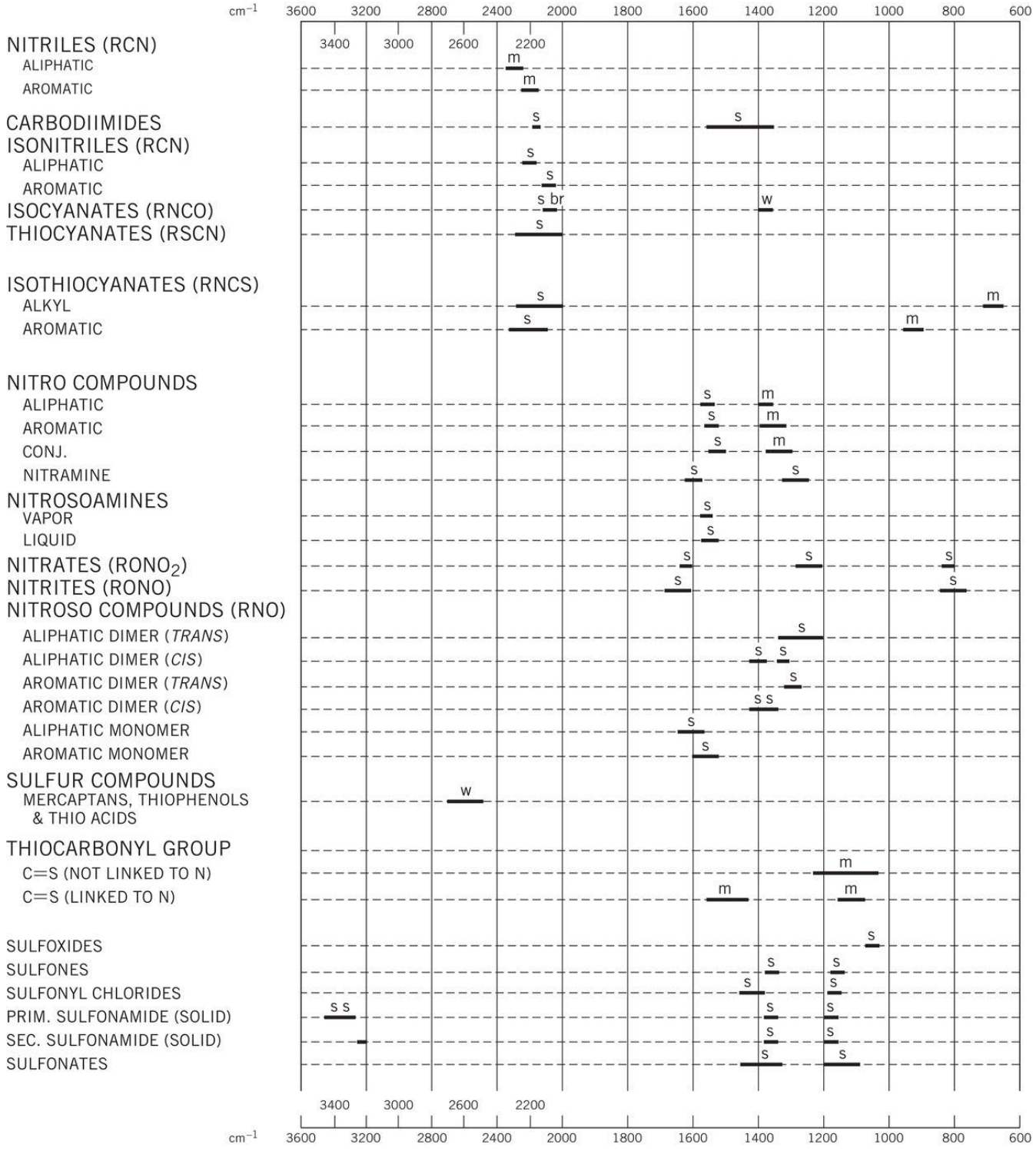


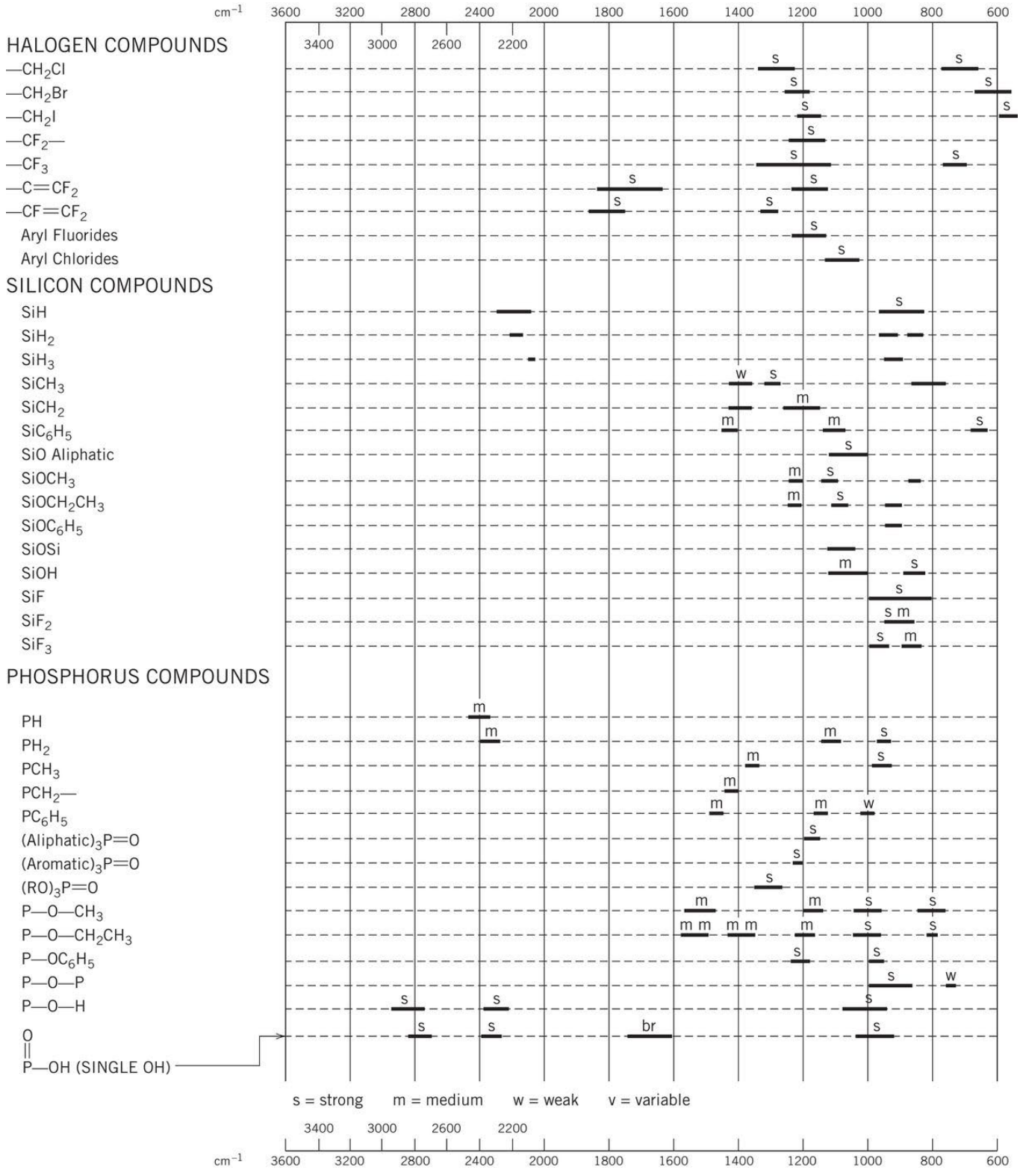
[a] Three bands, sometimes a fourth for ketals, and a fifth band for acetals.

[b] Conjugated aliphatic examples show C═O stretch at virtually the same position as aromatic structures.

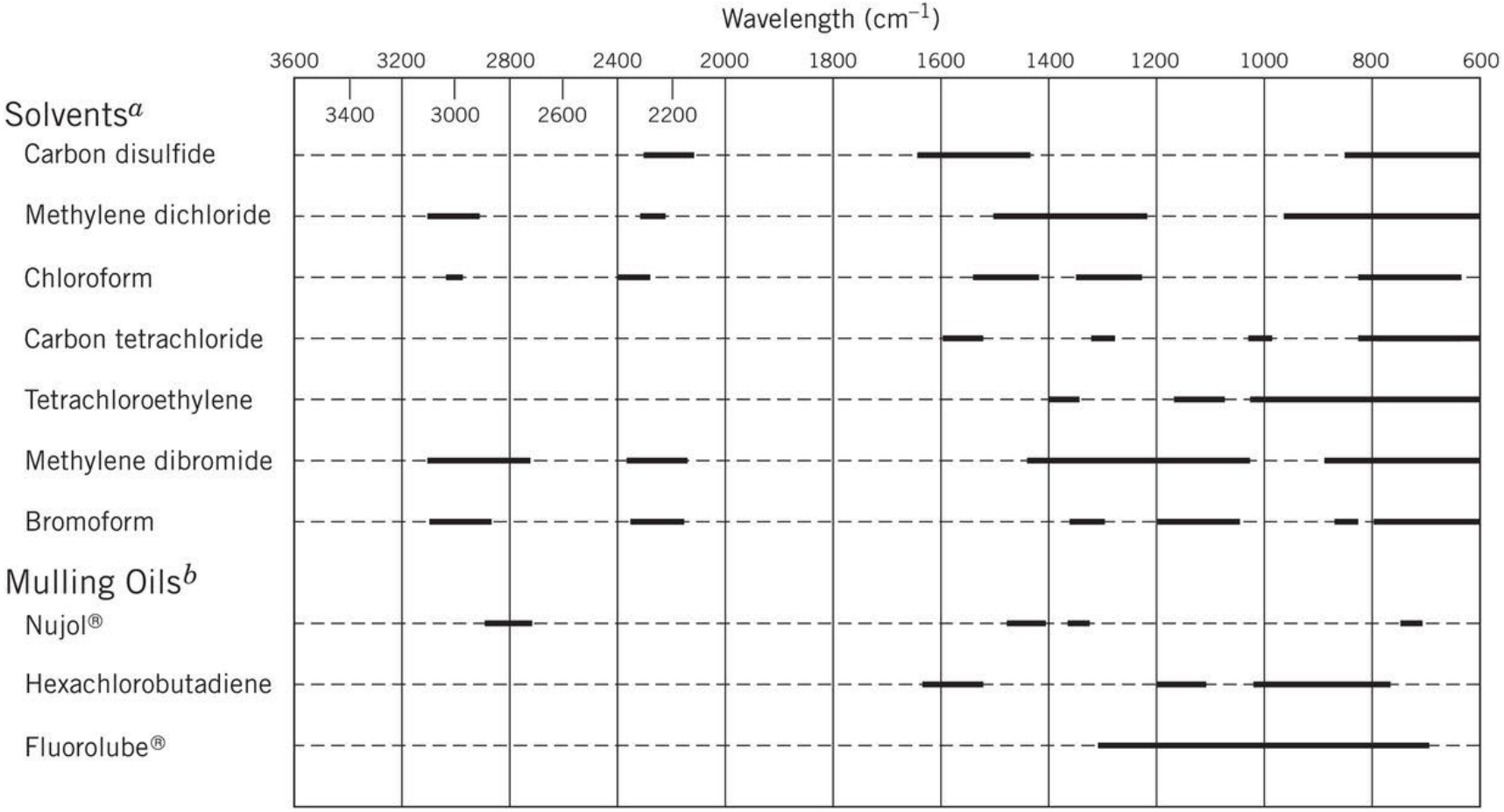
[c] Conjugated examples show C═O stretch at lower wavenumbers (1710 cm^{-1} to 1680 cm^{-1}). The O—H stretch (3300 cm^{-1} to 2600 cm^{-1}) is very broad.


cm⁻¹
3600 3200 2800 2400 2000 1800 1600 1400 1200 1000 800 600
3400 3000 2600 2200
LACTONES
BETA
GAMMA
DELTA
ACID CHLORIDES
ALIPHATIC
AROMATIC
ANHYDRIDES
NON-CYCLIC (UNCONJ)
NON-CYCLIC (CONJ)
CYCLIC (UNCONJ)
CYCLIC (CONJ)
AMIDES
PRIMARY
SOLUTION
SOLID
SECONDARY
SOLUTION
SOLID
TERTIARY
LACTAMS
SOLUTION
SOLID
5-MEMBERED RING
6 OR 7-MEMBERED RING
AMINES
PRIMARY
ALIPHATIC
AROMATIC
SECONDARY
ALIPHATIC
AROMATIC
TERTIARY
ALIPHATIC
AROMATIC
AMINE SALTS
PRIMARY
SECONDARY
TERTIARY
AMMONIUM ION


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 COMPOUNDS
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. SULFONAMIDE (SOLID)
SULFONATES


cm⁻¹ 3600 3200 2800 2400 2000 1800 1600 1400 1200 1000 800 600
3400 3000 2600 2200
HALOGEN COMPOUNDS
—CH2Cl
—CH2Br
—CH2I
—CF2—
—CF3
—C=CF2
—CF=CF2
Aryl Fluorides
Aryl Chlorides
SILICON COMPOUNDS
SiH
SiH2
SiH3
SiCH3
SiCH2
SiC6H5
SiO Aliphatic
SiOCH3
SiOCH2CH3
SiOC6H5
SiOSi
SiOH
SiF
SiF2
SiF3
PHOSPHORUS COMPOUNDS
PH
PH2
PCH3
PCH2—
PC6H5
(Aliphatic)3P=O
(Aromatic)3P=O
(RO)3P=O
P—O—CH3
P—O—CH2CH3
P—OC6H5
P—O—P
P—O—H
O
||
P—OH (SINGLE OH)
s = strong m = medium w = weak v = variable
3400 3000 2600 2200
cm⁻¹ 3600 3200 2800 2400 2000 1800 1600 1400 1200 1000 800 600

Transparent regions of solvents and mulling oils



[a] The open regions are those in which the solvent transmits more than 25% of the incident light at 1 mm thickness.

[b] The open regions for mulling oils indicate transparency of thin films.