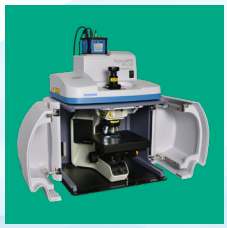
HORIBA

Raman

Raman Data and Analysis

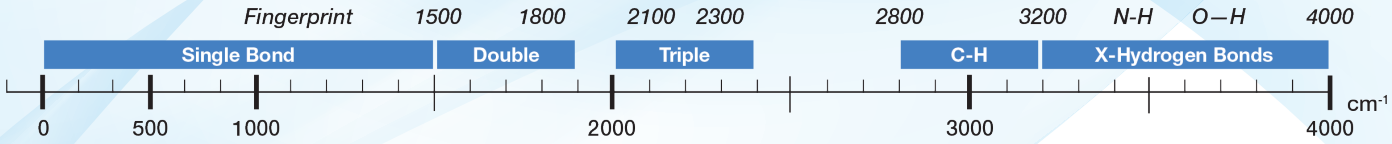


Technical Note
RA TN-18

Raman spectroscopy produces characteristic spectral bands that correspond to the vibrational modes of molecules within a sample. These bands provide valuable information about molecular composition and structure.

While the exact positions of these bands can vary depending on factors like sample composition and environment, below are some of the more common Raman band assignments.

Common Raman Bands



Functional Group/Vibration	Region	Raman
Lattice vibrations in crystals, LA modes	10 - 200 cm^{-1}	strong
δ(CC) aliphatic chains	250 - 400 cm^{-1}	strong
υ(Se-Se)	290 - 330 cm^{-1}	strong
υ(S-S)	430 - 550 cm^{-1}	strong
υ(Si-O-Si)	450 - 550 cm^{-1}	strong
υ(Xmetal-O)	150 - 450 cm^{-1}	strong
υ(C-I)	480 - 660 cm^{-1}	strong
υ(C-Br)	500 - 700 cm^{-1}	strong
υ(C-Cl)	550 - 800 cm^{-1}	strong
υ(C-S) aliphatic	630 - 790 cm^{-1}	strong
υ(C-S) aromatic	1080 - 1100 cm^{-1}	strong
υ(O-O)	845 - 900 cm^{-1}	strong
υ(C-O-C)	800 - 970 cm^{-1}	strong
υ(C-O-C) asym	1060 - 1150 cm^{-1}	strong

υ(CC) alicyclic, aliphatic chain vibrations	600 - 1300 cm^{-1}	medium	medium
υ(C=S)	1000 - 1250 cm^{-1}	strong	weak
υ(CC) aromatic ring chain vibrations	*1580, 1600 cm^{-1}	strong	medium
	*1450, 1500 cm^{-1}	medium	medium
	1000 cm^{-1}	strong/medium	weak
δ(CH3)	1380 cm^{-1}	medium	strong
δ(CH2) δ(CH3) asym	1400 - 1470 cm^{-1}	medium	medium
δ(CH2) δ(CH3) asym	1400 - 1470 cm^{-1}	medium	medium
υ(C-NO2)	1340 - 1380 cm^{-1}	strong	medium
υ(C-NO2) asym	1530 - 1590 cm^{-1}	medium	strong
υ(N=N) aromatic	1410 - 1440 cm^{-1}	medium	-
υ(N=N) aliphatic	1550 - 1580 cm^{-1}	medium	-
δ(H2O)	~1640 cm^{-1}	weak broad	strong
υ(C=N)	1610 - 1680 cm^{-1}	strong	medium
υ(C=C)	1500 - 1900 cm^{-1}	strong	weak
υ(C=O)	1680 - 1820 cm^{-1}	medium	strong
υ(C≡C)	2100 - 2250 cm^{-1}	strong	weak
υ(C≡N)	2220 - 2255 cm^{-1}	medium	strong
υ(-S-H)	2550 - 2600 cm^{-1}	strong	weak
υ(C-H)	2800 - 3000 cm^{-1}	strong	strong
υ(=C-H))	3000 - 3100 cm^{-1}	strong	medium
υ(≡C-H))	3300 cm^{-1}	weak	strong
υ(N-H)	3300 - 3500 cm^{-1}	medium	medium
υ(O-H)	3100 - 3650 cm^{-1}	weak	strong

It is important to note that Raman bands can vary depending on factors such as molecular symmetry, conjugation, and the presence of functional groups. Interpretation of Raman spectra often involves comparing observed bands to reference data and considering the specific molecular context.

Reference

Socrates, G. (2001). Infrared and Raman Characteristic Group Frequencies, Third Edition. John Wiley and Sons.

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