RAMAN DATA AND ANALYSIS

Raman Spectroscopy for Analysis and Monitoring

The Raman scattering technique is a vibrational molecular spectroscopy which derives from an inelastic light scattering process. With Raman spectroscopy, a laser photon is scattered by a sample molecule and loses (or gains) energy during the process. The amount of energy lost is seen as a change in energy (wavelength) of the irradiating photon. This energy loss is characteristic for a particular bond in the molecule. Raman can best be thought of as producing a precise spectral fingerprint, unique to a molecule or indeed and individual molecular structure. In this respect it is similar to the more commonly found FT-IR spectroscopy. However, unlike FT-IR, there are a distinct number of advantages when using Raman.

- *Raman can be used to analyse aqueous solutions since it does not suffer from the large water absorption effects found with FT techniques.*
- *The intensity of spectral features in solution is directly proportional to the concentration of the particular species*
- *Raman spectra are generally robust to temperature changes*
- *Raman requires little or no sample preparation. It does not need the use of Nujol, or KBr matrices and is largely unaffected y sample cell materials such as glass.*
- *The use of a Raman microscope such as the LabRAM provides very high level of spatial resolution and depth discrimination, not found with the FT methods of analysis*

These advantages and its highly specific nature, mean that Raman has become a very powerful tool for analysis and chemical monitoring. Depending upon instrumentation, it is a technique which can be used for the analysis of solids, liquids and solutions and can even provide information on physical characteristics such as crystalline phase and orientation, polymorphic forms, and intrinsic stress.

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

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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$\cong$C)	2100 - 2250 cm^{-1}	strong	weak
υ(C$\cong$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($\cong$(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

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