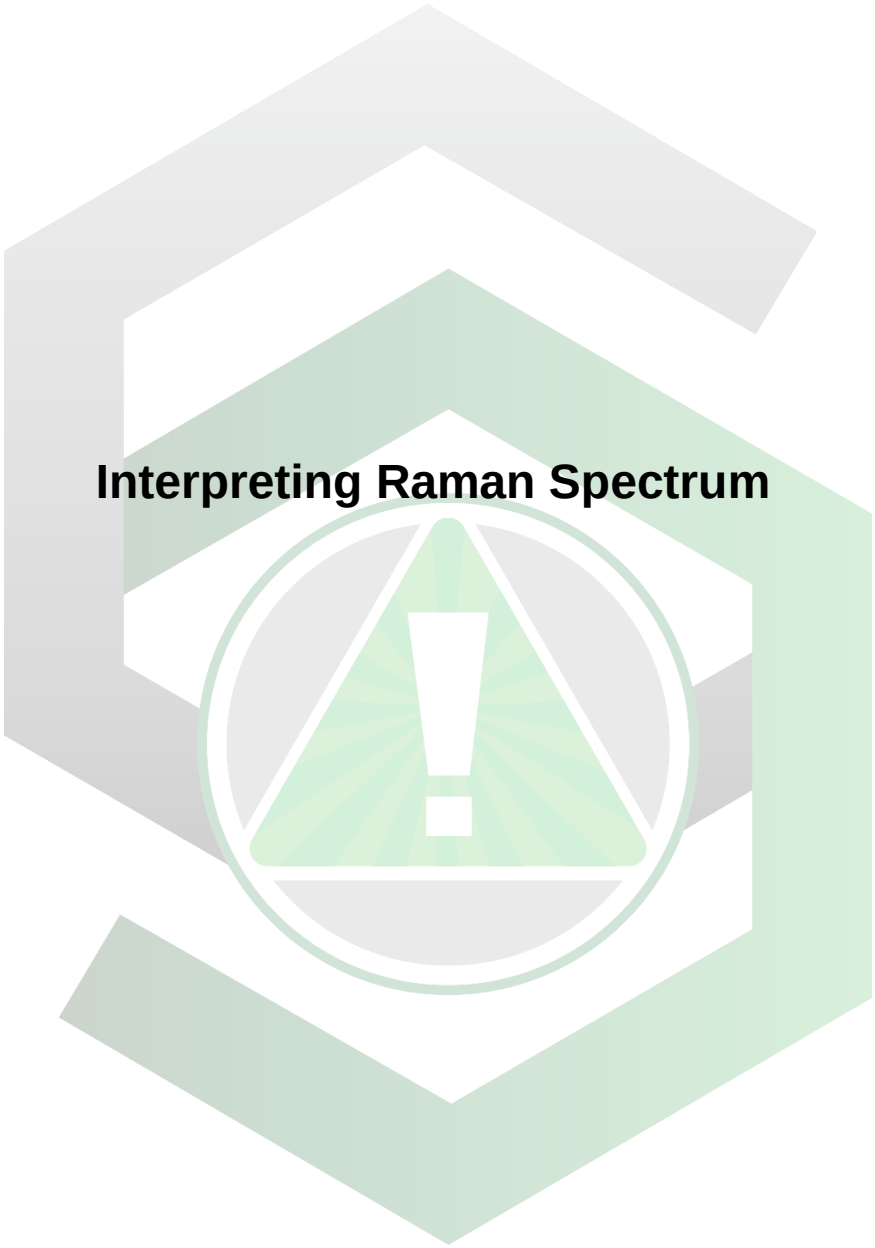
Interpreting Raman Spectrum



Created by: Edwin Caballero-Agosto

Manager: Samuel Hernandez-Rivera

SOP-01	**Edwin Caballero Agosto**		**University of Puerto Rico at Mayagüez**
Effectivity: 9/18/2021	**Interpreting Raman Spectrum**		**Revised by:**
Revised:			**Approved by:**

INTERPRETING RAMAN SPECTRUM

SAMPLE AND PREPARATION EFFECTS

1. What is the name of the sample?

---

2. Instrument information:

Name: _____

Laser: _____

Excitation wavelength: _____

Spectral Range: _____

Spectral Resolution: _____

3. How was the sample produced?

---

4. What is known of the reaction scheme?

---

5. Are there possible side reactions?

---

6. Could solvents be present?

---

7. Did work-up conditions introduce impurities?

---

8. State of matter.

☐ Solid:

Dry ☐ , Paste ☐ ,

Was it washed with solvent or recrystallized? Yes ☐ No ☐ ,

Neat ☐ , Halide disk ☐ , Mull ☐ , Neat powder ☐

☐ Liquid:

Volatile ☐ , Alkaline ☐ , Neutral ☐ , Acidic ☐ , Pure liquid ☐ , Solution ☐

☐ Gas:

Temperature

Pressure

Purity

Elemental info

Contain N, S, or halogens ☐,

Could the N, S or halogens be from impurity? Yes ☐ No ☐ ,

Polarization Effects ☐ , Orientation Effects ☐ , Temperature Effects ☐

9. If sample is in container:

Mark off bands due to vessel walls (e.g., glass, polythene).

In cast or polymer films, is there any solvent trapped or encapsulated?

Can the polymer film have orientation?

---

10. If Raman is paired with microscope.

Are the bands real or due to the mounting window (e.g., diamond).

INSTRUMENT AND SOFTWARE EFFECTS

1. Are resonance or self-absorption likely to affect band strengths? Yes ☐ , No ☐

2. Does the spectrum have: Flat background ☐ , Corrected for fluorescence ☐

3. Did software used smooth function? Yes ☐ , No ☐

4. Are the broad band in the spectrum due to: Fluorescence ☐ , Burning ☐ , Other ☐

5. Are the sharp bands in the spectrum due to: Cosmic rays ☐ , Neon room lights ☐ , Other ☐

MAIN INTERPRETATION

1. Is a reference spectrum available? Yes ☐ , No ☐

2. Does the total spectrum look like the reference spectrum? Yes ☐ , No ☐

3. Hit Quality Index between sample and reference:

---

4. Correlation coefficient between sample and reference:

---

5. Are the bands: Broad ☐ , Sharp ☐ , Strong ☐ , Weak ☐

6. Is the background: Sloping ☐ , Flat ☐

7. In the 3600-3100 cm^{-1} region are there: -OH ☐ , -NH ☐ bands. Look for related bonds for confirmations (e.g., amides have carbonyl bands and -NH bands).

	NAME	STRENGTH	REGION [cm^{-1}]	
☐	Thiols (SH)	m	2531	2615
☐	Aldehydes 1	m	2684	2741
☐	N-CH3	m	2753	2797
☐	CH2 1	s	2766	2838
☐	Aldehydes 2	w	2782	2838
☐	O-CH3	m	2782	2838
☐	C-CH3	s	2817	2958
☐	OH	w	2876	3534
☐	CH2 2	s	2892	2935
☐	Aromatic C-H	s	2973	3086
☐	CH=CH	s	2976	3032
☐	=CH2	s	3017	3073
☐	Amine, Amide	m	3152	3470
☐	Phenol	m	3211	3406
☐	Alcohol	m	3224	3337
☐	Alkyne	w	3242	3285

8. In the 3200-2700 cm^{-1} region are there: Unsaturation ☐ , Aliphatic ☐ bands. Usually unsaturation is above 3000 cm^{-1} and aliphatics below.

If aliphatic bands are present, are they largely: Methyl ☐ , Longer -CH2 ☐ groups.

Are the bands in the cumulative bond region 2700-200 cm^{-1}? Yes ☐ , No ☐

Are there bands in the double bond (e.g., -C=O, -C=C) region 1800-1600 cm^{-1}? Yes ☐ , No ☐

	NAME	STRENGTH	REGION [cm^{-1}]	
☐	Carboxylic Acid	m	1687	1737
☐	Ketone	m	1692	1719
☐	Aldehyde	m	1700	1727
☐	Ester	m	1708	1745
☐	Lactone	m	1735	1793
☐	Acid chloride	m	1740	1788
☐	Anhydride	m	1748	1838
☐	Isothiocyanate	m	2019	2090
☐	Alkyne	s	2058	2242
☐	Si-H	m	2074	2146
☐	Isonitrile	m	2088	2173
☐	Thiocyanate	w	2101	2173
☐	Azide	m	2117	2159
☐	Diazonium salt	m	2199	2284
☐	Aromatic nitrile	m	2199	2228
☐	Nitrile	m	2226	2255
☐	Isocyanate	w	2226	2271
☐	P-H	w	2295	2425
☐	Thiols (SH)	s	2531	2616

9. In the 1700-200 cm^{-1} region are there:

Many bands largely due to the molecule fingerprint? Yes ☐ , No ☐

1700-1200 cm^{-1}

	NAME	STRENGTH	REGION [cm^{-1}]	
☐	Sulphonic acid 1	w	1196	1243
☐	Carboxylate salt	m	1313	1431
☐	Nitro 1	s	1320	1355
☐	C-CH3	m	1358	1386
☐	Aromatic azos	s	1367	1445
☐	CH2, CH3	m	1409	1458
☐	Aromatic ring	m	1451	1507
☐	Nitro 2	m	1534	1605
☐	Aliphatic azos	m	1541	1590
☐	Amide	s	1555	1695
☐	Aromatic/hetero ring	s	1555	1612
☐	Ketone	m	1604	1715
☐	Carboxylic acid	m	1612	1723
☐	C=C	s	1618	1674
☐	C=N	s	1625	1667
☐	Urethane	m	1688	1716
☐	Aldehyde	m	1715	1737
☐	Aliphatic ester	m	1729	1764

1200-700 cm^{-1}

	NAME	STRENGTH	REGION [cm^{-1}]	
☐	ν C-C aliphatic chains	m	700	1263
☐	CHX=CYZ	m	887	992
☐	C-Cl	s	701	785
☐	C-S	s	707	777
☐	C-F	s	722	805
☐	C-O-C Ethers	m	798	951
☐	Carboxylic acid dimer	m	909	959
☐	Aromatic rings	s	992	1102
☐	Si-O-Si, Si-O-C	m	1006	1089
☐	C=S	s	1013	1228
☐	Sulphonic acid 2	m	1020	1063
☐	Sulphone sulphonamide	m	1049	1207
☐	Si-O-C	m	1117	1187
☐	Sulphonic acid 1	m	1144	1261

700-200 cm^{-1}

	NAME	STRENGTH	REGION [cm^{-1}]	
☐	Lattice vibrations	s	47	210
☐	Xmetal-O	s	128	435
☐	δ C-C aliphatic chains	s	254	401
☐	Se-Se	s	294	340
☐	S-S	s	427	543
☐	Si-O-Si	s	457	552
☐	C-I	s	485	658
☐	C-Br	s	507	700
☐	C-Cl	s	550	765
☐	C=S	s	571	673
☐	ν C-C aliphatic chains	m	622	765
☐	C-S aliphatic	s	666	754

OVERALL RESULTS

Confirmed?	Bands	Region	NAME
☐	1		
☐	2		
☐	3		
☐	4		
☐	5		
☐	6		
☐	7		
☐	8		
☐	9		
☐	10		
☐	11		
☐	12		
☐	13		
☐	14		
☐	15		
☐	16		
☐	17		
☐	18		
☐	19		
☐	20		
☐	21		
☐	22		
☐	23		
☐	24		
☐	25		
☐	26		
☐	27		
☐	28		
☐	29		
☐	30		
☐	31		
☐	32		
☐	33		
☐	34		
☐	35		
☐	36		

Advisor Signature

_____

Co-Advisor Signature

_____