CHARISMA

Guide to Collecting Good Raman Data

While the initial concept of Raman spectroscopy is in itself simple (excite the sample with a laser and collect the scattered light), ensuring good data can be more complex. Below are some hints to help.

Safety first

- Observe laser safety procedures – Wear laser glasses or use an enclosure.
- Instrument software can be very complex, if you do not understand a setting, do not change it. Use preselected setup to get started.
- Beware of dark and colourful samples – they absorb laser and can heat or BURN. Start at a low laser power and work up.
- Make sure the sample is in laser focus – not always the same as visual focus.
- Single point or mapping – mapping requires the sample to be flat across the plane of analysis.
- Freedom of movement – if the sample is very uneven, make sure the lens is safe to move around and find focus.

Know your instrument

- Check optics for smudges/contamination – these can interfere with the incoming signal.
- Interlocks engaged, and shutters open – if the laser cannot reach the sample, no Raman scatter can be induced.
- Let the laser warm up – stable lasers will give reproducible results.
- Laser drift – input power or laser temperature can affect the laser wavelength, and drift can occur over time.
- Optical alignment issues – in free space laser systems, differences in the alignment can change the spectrum.
- Verify the calibration using a reference material.

Know your sample

- What is the expected spectrum? – Does a database example of your sample's spectrum exist, so you know what you expect to see?
- Fluorescence – will your sample have fluorescence; can you analyse with an IR or UV laser to mitigate it?
- Heating – will your sample heat with laser exposure?
- Photo-bleaching – will the fluorescence reduce with continued exposure to the laser?
- Dehydration – will the changes in the water content of the sample alter the spectrum observed?

Check your data

- Check for the saturation – reduce the laser power or exposure time to prevent saturation.
- Signal to noise – are all your peaks of interest clearly visible above the noise?
- A background measurement is best practise – removes environmental lights and detector behaviours from spectra. Light blocking enclosures can reduce the background light, but this should not replace background subtraction.
- Sample holder interference – use hollow holders or avoid black holders.
- Include metadata – Information on the acquisition parameters & conditions, instrument, sample, and operator should be included with the spectrum file for future reference.

Conclusion

If you have a full understanding of your instrument's behaviour, and keep in mind the hints above with every spectrum, you will always have good, usable Raman data.

CHARISMA's contribution

A goal of CHARISMA is to create tools for FAIR (Findable Accessible Interoperable Reusable) Raman data. Ensuring a high quality of the Raman spectra to be presented in this FAIR format is extremely important.

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