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Stimulated versus spontaneous Raman spectroscopy for trace-level detection of minority species in aqueous solutions

Environmental regulations are driving the need to detect minority species in aqueous solutions at increasingly low concentrations. Raman spectroscopy is well suited to this task, working directly with aqueous samples and providing both qualitative and quantitative information without sample preparation. Its main limitation, however, is the inherently weak Raman scattering cross-section. Here, we compare the limit of detection of nitrate in water using spontaneous Raman spectroscopy and stimulated Raman scattering [1,2], the latter realized with a tunable picosecond laser (Picus Duo), balanced detection, and lock-in amplification.

We clarify when each method is preferable: spontaneous Raman for its simpler instrumentation and broad spectral coverage, and stimulated Raman at low concentrations and against a strong aqueous background, where it offers higher signal levels. We present calibration data and detection limits, evaluate signal linearity at low concentrations, and demonstrate a custom denoising pipeline that suppresses the dominant aqueous background, lowering the detectable concentration towards the (sub)-ppm regime.

Acknowledgement

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References

- [1] K. J. Mohn, B. Dong, S. Mahapatra, I. K. Singh, J. P. Lomont, B. Wan, C. Zhang, Journal of Physical Chemistry B, 2025, 9446-9456, 129
- [2] R. C. Prince, R. R. Frontiera, E. O. Potma, Chemical Reviews, 2017, 117

Figures

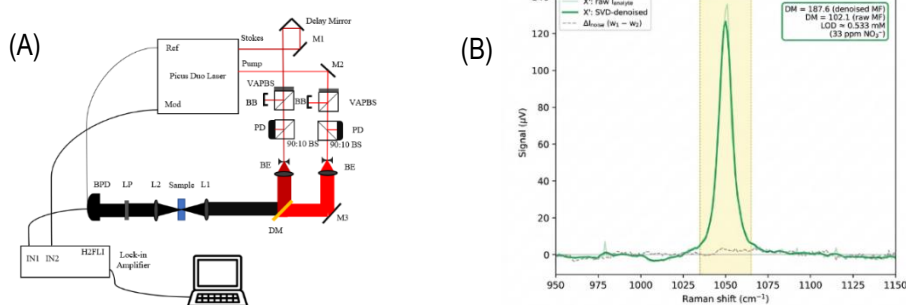


Figure 1: (A) Schematic overview of the SRS instrument setup detailing the optical routing of the laser to the sample and signal acquisition via a balanced photodetector (BPD) and lock-in amplifier. (B) Spectral evaluation from the latest run showing the stimulated Raman signal of 100 mM KNO₃; SVD denoising and matched filtering yield an optimal limit of detection of 0.533 mM (33 ppm NO₃⁻).