Ramdb: The NASA Raman Spectral Database (version 1.00)

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Given that, in most instances, minimal sample preparation is required and due to its contactless instrument design, Raman spectroscopy is one of the most versatile vibrational spectroscopic techniques for the chemical analysis of environmental and biological specimens. The diversity of applications of Raman spectroscopy ranges anywhere from art [1] to planetary science missions [2]. The advancement in the use of Raman spectroscopy in Solar System missions, notably in post-mission sample return analysis, requires a spectral library holding the broad range of specimens that could be found in Solar System sources. For this purpose, we have initiated the development of a Raman spectral database (Ramdb) at NASA Ames Research Center. Currently, the database includes experimental and theoretical Raman spectra of PAHs [3, 4], as well as laboratory Raman spectra of amino acids, carbon allotropes, minerals, and analogs relevance to Earth Sciences [5], Exobiology [6], Planetary [7], and Astrochemistry [8] to name just a few examples. Ramdb can be found on the web at www.astrochemistry.org/ramdb, where raw and processed Raman spectra can be downloaded in CSV format.

The laboratory Raman spectra are measured using a laser Raman spectrometer (JASCO NRS-5500-532QRI). The Raman instrument is equipped with three excitation lasers, with wavelengths of 405, 532, and 785 nm. A clean silicon substrate is used as the internal standard for wavenumber calibration. Powdered samples were prepared (microscopic >10 um, grounded microscopic < 10 um) on glass slides. Some raw data exhibited a background signal arising as a combination of laser-induced fluorescence from the sample. To correct this background, we developed a Python pipeline that uses open-source Python libraries. Ramdb provides both raw and processed (using Python pipeline) data, which includes tabulated Raman shift transitions and other measurement details. The theoretical Raman band positions of PAHs (pyrene monomers and tetramer clusters) were computed using density functional theory (DFT) with the help of the Gaussian 16 suite of programs [9].

In the near future, Ramdb will serve as a repository of Raman spectral data from Laboratory Astrophysics and Planetary Science experiments involving the irradiation of organic compounds under simulated space and planetary conditions. In addition, online and offline tools will be developed for utilising the database for comparison to the user's sample.

References

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