Hunting elusive molecules with rotational spectroscopy

Rotational spectroscopy is an invaluable tool to unambiguously determine the molecular structure of a species, and sometimes even to establish its very existence. The laboratory detection of molecules often relies on the close and mutually beneficial interaction between high-level theoretical calculations and sensitive rotational measurements. Using the example of gauche-butadiene, I will illustrate how state-of-the-art experimental tools, used in tandem with high-level theoretical calculations, can enable the detection of elusive molecules.

Perhaps the most elusive species are those existing in rich chemical mixtures, of unknown exact composition, as often encountered on Earth or in the interstellar medium. There again, beyond the detection of targeted molecules and because of its structural specificity, rotational spectroscopy has great potential as an analytical tool for characterizing the chemical composition of complex gas mixtures. We have developed an experimental methodology to perform unbiased searches for novel molecules in the laboratory. This procedure, called spectral taxonomy, involves acquiring a broadband rotational spectrum of a rich mixture, categorizing individual lines based on their relative intensities under series of assays, and finally, linking rotational transitions of individual chemical compounds within each category using double resonance techniques. I will illustrate the power of this procedure, initially developed in the centimeter-wave domain and currently being implemented in the submillimeter region, through several examples of either (or both) chemical or astronomical interest.