IDENTIFYING BROADBAND ROTATIONAL SPECTRA WITH NEURAL NETWORKS

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A typical broadband rotational spectrum may contain several thousand observable transitions, spanning many species[a]. Identifying the individual spectra, particularly when the dynamic range reaches 1,000:1 or even 10,000:1, can be challenging. One approach is to apply automated fitting routines[b]. In this approach, combinations of 3 transitions can be created to form a "triple", which allows fitting of the A, B, and C rotational constants in a Watson-type Hamiltonian. On a standard desktop computer, with a target molecule of interest, a typical AUTOFIT routine takes 2–12 hours depending on the spectral density. A new approach is to utilize machine learning[c] to train a computer to recognize the patterns (frequency spacing and relative intensities) inherit in rotational spectra and to identify the individual spectra in a raw broadband rotational spectrum. Here, recurrent neural networks have been trained to identify different types of rotational spectra and classify them accordingly. Furthermore, early results in applying convolutional neural networks for spectral object recognition in broadband rotational spectra appear promising.

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[a] Perez et al. "Broadband Fourier transform rotational spectroscopy for structure determination: The water heptamer." Chem. Phys. Lett., 2013, 571, 1–15.

[b] Seifert et al. "AUTOFIT, an Automated Fitting Tool for Broadband Rotational Spectra, and Applications to 1-Hexanal." J. Mol. Spectrosc., 2015, 312, 13–21.

[c] Bishop. "Neural networks for pattern recognition." Oxford university press, 1995.