ANALYSIS OF MICROWAVE-MICROWAVE DOUBLE RESONANCE SPECTRA WITH CONVOLUTIONAL NEURAL NETWORKS

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Microwave-microwave double resonance (MMDR) spectroscopy is a type of two-dimensional spectroscopy that identifies pairs of rotational transition frequencies that share a quantum state. MMDR spectra are an effective tool for identifying transition ladders in a rotational spectrum, and, qualitatively, they can provide insight into molecular asymmetry and the strength of cartesian dipole components[a]. In this work, a set of convolutional neural network (CNN) classification and regression models are trained to predict non-zero dipole components and ratios of principal rotational constants from MMDR spectra. Like many deep learning methods, training CNN models requires a large set of labeled training data which precludes their usefulness in many spectroscopy applications. Here, the CNNs are trained on datasets of simulated rigid rotor MMDR spectra created with Pickett's SPCAT and randomly generated sets of the principal rotational constants: A, B, and C. Preliminary results show that, with a sufficiently dense MMDR spectrum, the models frequently predict the correct non-zero dipole components and can determine the C/B and C/A ratios with RMSEs of 0.1 and 0.05.

[a]Martin-Drumel et al. 2016 JCP 144, 124202