AUTOMATED ASSIGNMENT OF ROTATIONAL SPECTRA USING ARTIFICIAL NEURAL NETWORKS

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Last year at this conference several approaches to utilize machine learning[a] to train a computer to recognize the patterns inherit in rotational spectra were presented[b]. It was shown that the recognized patterns could be used to identify (or classify) a rotational spectrum by its Hamiltonian type, but at the time, the rotational constants were not recovered. Here, we describe a feed forward artificial neural network that has been trained to identify different types of rotational spectra and determine the parameters of the molecular Hamiltonians. The network requires no user interaction beyond loading a "peak pick", and can return fits within a fraction of a second. The rotational constants are typically deduced with the accuracy of 1–10 MHz. We will describe how the network works and provide benchmarking results.

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[a] Bishop, C M. "Neural networks for pattern recognition." Oxford university press, 1995.

[b] Zaleski, D. P.; Prozument, K. Identifying Broadband Rotational Spectra with Neural Networks, International Symposium on Molecular Spectroscopy, June 21; 2017.