GAS-PHASE INFRARED SPECTRA ANALYSIS VIA DEEP NEURAL NETWORKS

ABIGAIL A ENDERS, NICOLE NORTH, HEATHER C. ALLEN, *Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH, USA*.

Infrared spectroscopy provides unique molecular vibrational information that is molecule and environment specific. Spectral responses, as images rather than array-based data, were used to train a deep neural network to develop analytical methods capable of large-scale information processing. We label spectra based on the present and absent functional groups, but the model must determine the frequencies, peak shape, and variability of each molecular response to identify functional groups. The resultant machine learning models significantly reduce the time required for traditional infrared spectral analysis and the functional group assignments is found to be more accurate than expert chemists. Application of machine learning methods to spectroscopic data is made approachable by a straightforward model system that is generalizable, broad, and well-performing on thousands of gas-phase infrared spectra from the NIST spectral database. Future improvement will involve more specific and applied models, such as the investigation of field samples for environmental contaminants or component identification, with increased solvent complexity to continue developing a broad range of models. To the best of our knowledge, this is the first presentation of a generalizable machine learning model for infrared analysis because it is capable of analyzing a diverse spectral database.