IMPLEMENTING EXTENDED CROSS CORRELATION AS A TOOL FOR SEMI-AUTOMATED MICROWAVE SPECTROSCOPIC ANALYSIS OF WEAKLY BOUND CLUSTER SPECTRA

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Rapid recording of molecular spectra of complex mixtures has facilitated acquisition of high sensitivity data sets. In studies of weakly bound clusters, these spectra may contain a wide range of cluster sizes and abundances, leading to intensities spanning many orders of magnitude between the strongest and weakest spectra present. The line densities and wide dynamic ranges of these high sensitivity spectra often lead to bottlenecks at the spectroscopic assignment and analysis stages of an experiment. Recent developments in artificial intelligence and machine learning have the potential to lead to fast, automated approaches to the spectroscopic assignment process. Here, we present an implementation of Jacobson, *et al*'s extended cross correlation (XCC) approach[a] to separating transitions arising from different species. While not leading to fully automated spectroscopic assignment on its own, XCC provides simplified data sets that can be more easily analyzed by visual pattern recognition or combined with other automated approaches. Initial XCC results will be compared with our previous implementation of principal component analysis-based examination of microwave spectra of complex mixtures of fluorinated ethylene/CO_2 clusters. In addition to simplifying raw datasets, these semi-automated analyses may provide insights that help identify the species present in the mixture, as well as helping guide searches for spectra of new species.

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[a]M.P. Jacobson, S.M. Coy, R.W. Field, Extended Cross Correlation: A Technique for Spectroscopic Pattern Recognition, *J. Chem. Phys.* 107 (1997) 8349–8356.