PATTERN RECOGNITION BY EXTENDED AUTO- AND CROSS-CORRELATION

STEPHEN L. COY, MATTHEW P. JACOBSON, AND ROBERT W. FIELD, *Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139.*

The traditional approach to understanding the information encoded in spectroscopic data has been first to assign each transition observed and then to relate the positions and intensities of the transitions to a model that allows insight into the system being studied. In complex and congested spectra, however, the process of assignment may be difficult, tedious, or even impossible. In such a situation, it is often desirable to be able to recognize patterns that are obscured by the complexity of the spectrum. For this purpose, we have developed two closely related pattern recognition techniques, which we refer to as Extended Autocorrelation (XAC) and Extended Cross-Correlation (XCC). The XAC can be used to locate patterns that are parameterized in a complex way within a congested spectrum. The XCC recognizes patterns that are common among two or more spectra. Tests of these techniques using synthetic spectra will be presented, as well as applications to the mass spectra of large molecules (XAC) and FTIR spectra of mixtures of deuterated ammonia isotopomers (XCC).