DISENTANGLING VIBRATIONAL BANDS IN INFRARED SPECTRA OF CO BY UTILIZING SPECTROSCOPIC PATTERN RECOGNITION TECHNIQUES.

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Recently we have reported a novel pattern recognition technique entitled Extended Cross Correlation (XCC) which may be used to identify spectroscopic patterns in multiple spectra. The simplest application of this technique is to multiple spectra of mixtures of chemical species: the XCC can be used to identify which features in the spectra correspond to which chemical species. However the technique is applicable whenever a set of spectra may be described accurately as a linear superposition of spectroscopic "patterns", whether these patterns represent different chemical species, vibrational bands, polyads, etc. Here we report the application of the XCC to infrared spectra of highly vibrationally and rotationally excited carbon monoxide observed in atmospheric simulation experiments performed in the LABCEDE facility at the Phillips Laboratory. These complex and congested CO spectra were partially self-absorbed, making a complete analysis using conventional least-squares fitting techniques impossible. A novel combination of XCC and least-squares fitting has permitted a complete analysis of the data, providing an intriguing example of how pattern recognition techniques can be used when spectra contain spectroscopic patterns that are not known a priori.