STRATEGIES FOR INTERPRETING HIGH RESOLUTION COHERENT MULTIDIMENSIONAL SPECTRA

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The electronic spectra of certain molecules can be very complex and consist of a high density of peaks. The high density of peaks results in severe spectral congestion, making conventional data analysis techniques extremely difficult to use. One solution to this problem is to use high resolution coherent 2D spectroscopy (HRC2DS), which can improve resolution and sort peaks into recognizable clusters. This technique requires new data analysis techniques to accurately assign peaks. Even though HRC2DS can improve spectral resolution, some regions of the spectra may still remain congested. The ability to solve this problem using even higher dimensional techniques (e.g., high resolution coherent 3D spectroscopy) with 3D pattern recognition and data analysis techniques will be discussed.