IMPROVEMENT OF THE ANALYSIS OF THE PEROXY RADICALS USING AN EVOLUTIONARY ALGORITHM

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For quite awhile, our laboratory has had interest in the organic peroxy radicals which are relevant to atmospheric chemistry as well as low temperature combustion. We first studied these radicals via room temperature cavity ringdown spectroscopy (CRDS). We continued our investigation of the same radicals using a quasi-Fourier-transform laser source using a supersonic jet expansion in order to obtain partially rotationally resolved spectra which are nearly doppler limited. In order to analyze our spectra we decided to complement our conventional least-square-fit method of simulating spectra by using a evolutionary algorithm (EA) approach which uses both the frequency and the intensity information that are contained in our dense and complicated spectra. This presentation will focus on the $CD_3O_2$ spectrum to demonstrate the capabilities and the quality of the fits obtained via the EA method and compare it with the traditional least-square-fit method.