COMPUTATIONAL STUDY OF THE POSSIBLE CONFOMERS OF THE PENTOXY RADICAL TO AID IN THE VIBRONIC ASSIGNMENT OF JET-COOLED ALKOXY RADICALS

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We have recently obtained the jet-cooled spectra of the $\tilde{B} \leftrightarrow \tilde{X}$ transition of a number of alkoxy radicals containing from 3-12 carbon atoms. Assignment of the various bands observed is a challenge. In particular fairly intense low frequency bands (330 cm^{-1} for the 1-alkoxy radicals, and $\sim$140 cm^{-1} for the 2-alkoxy radicals) exhibit a rotational contour markedly different from that of the origin band. A possible explanation for the different contours is the presence of more than one conformer in the jet. To assess this possibility, calculations were performed on a number of conformers of the 1-, 2-, and 3-pentoxy species. These calculations were done at a density functional theory level to obtain the relative energies as well as rotational constants for the various conformers. During this talk we will discuss the possible conformers and how these results are being applied to the analysis of the various vibronic bands found in the spectra.