JET-COOLED LIF SPECTROSCOPY OF 2-BUTOXY RADICAL

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Combustion of fossil fuels and decomposition of hydrocarbon species injected into the atmosphere are obviously important chemical processes. Alkoxy radicals are important intermediates in these reactions. Recently we reported the analysis of the rotational structure of the $\tilde{B}$-$\tilde{X}$ electronic transition of a large number of primary alkoxy radicals, 1-$C_nH_{2n+1}O$. For this class of molecules (n>2), a complicated PES with multiple minima permits different conformational structures for each molecule, which could be reflected in their spectra. The rotational analysis of these spectra requires inclusion of the interaction of the unpaired electron on the p-orbital of oxygen with the rotation of the molecule (spin-rotation). The spin-rotation tensor elements together with the rotational constants of the molecule become a unique "fingerprint", i.e., a set of data identifying not only the molecule but also its specific geometric conformation. We have now turned our attention to the secondary alkoxy isomers. High resolution (250MHz) $\tilde{B}$-$\tilde{X}$ LIF spectra of 2-butoxy (2-C_4H_9O) have been recorded under jet-cooled conditions. The origin band of the most stabile conformer of 2-butoxy was analyzed, the observed rotational constants being consistent with *ab initio* calculations of its geometric structure. Values for the spin-rotation tensor are correlated with the results from previously studied primary alkoxies. The strong CO-stretch excitation band, normally very bright in primary alkoxies appears broadened, which may be taken as evidence for strong coupling of the CO stretch in the excited $\tilde{B}$ state with other states of 2-butoxy.