CONFORMATIONAL ASSIGNMENTS OF ROTATIONALLY RESOLVED SPECTRA OF 1-HEXOXY AND 1-HEPTOXY

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In recent work we have used ab initio calculations and rotational analyses to make conformational assignments for a number of bands in the laser induced fluorescence (LIF) spectra of the 1-propoxy, 1-butoxy and 1-pentoxy radicals. For larger alkoxy radicals (number of carbon atom greater than 5), the number of conformers becomes so great and the rotational structure so complex, that this method is very time-consuming and unattractive. Rather than pursue detailed rotational analysis of the 1-hexoxy and 1-heptoxy spectra we have made conformational assignments to individual spectra lines by using a guide the corresponding conformational assignments of smaller alkoxy radicals and their rotational constants and parameters from ab initio calculations. Refined assignments were made by using the GUI program SpecView.