CONFORMATIONAL ANALYSIS OF THIODIGLYCOL AND 2-HYDROXYETHYL ETHYL SULFIDE

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Last year at this meeting, we presented the conformational analysis of ethyl sulfide.[a] Here we report on the conformational analysis of two similar species, thiodiglycol (TDG) and 2-hydroxyethyl ethyl sulfide (HOEES) that are hydrolysis products found in the degradation of mustard gas. These studies are aimed at developing a rotational database to enable Fourier transform microwave (FTMW) spectroscopy to be used as a detection technique for chemical compounds related to chemical weapons (CW) technology. In addition to their importance in CW analysis, they present interesting spectroscopic problems as might be envisioned for single-bonded compounds with hydroxyl groups terminating the chain. Accordingly, we have identified three conformational isomers for TDG and two for HOEES in the gas phase. Details of the rotational analysis using a new interactive assignment program will be given. In addition, a comparison will be made between the observed and ab initio-calculated conformational structures.

[a]Talk TD11