ROTATIONAL SPECTRA AND STRUCTURES OF THE MUSTARD GAS PRECURSORS; DIVINYL SULFONE, DIVINYLSULFOXIDE, AND DIVINYL SULFIDE

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The rotational spectra of the three mustard gas (ClCH2CH2SCH2CH2Cl) precursors, divinyl sulfone (CH2CHS(O)2CHCH2), divinyl sulfoxide (CH2CHS(O)CHCH2), and divinyl sulfide (CH2CHSCHCH2) have been observed and analyzed using the mini FT spectrometer in the Edgewood Chemical and Biological Center Laboratory at Aberdeen, MD. All compounds are liquids at room temperature but all have sufficient vapor pressure to be observed using a reservoir nozzle at room temperature. The flexible nature of the heavy atom backbone in these species leads to the possibility of multiple conformers in the vapor phase. Indeed, for each species, the spectra from two conformational isomers have been observed and analyzed. Structural comparisons will be made within the series as well as comparison between the experimentally observed conformers and those determined from high level theoretical calculations.