ROTATIONAL SPECTRA, NUCLEAR QUADRUPOLE HYPERFINE AND CONFORMATIONAL STRUCTURES OF THE MUSTARD GAS SIMULENT CHLOROETHYL ETHYL SULFIDE

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Rotational spectra have been recorded for both the $^{35}$Cl and $^{37}$Cl isotopes of two structural conformations of chloroethyl ethyl sulfide (CEES); CEES differs from mustard gas (1,1-thiobis(2-chloroethane)) by only one chlorine on the thioethyl groups. The rotational constants of the two chlorine isotopomers were used to identify the conformations as GGT and TGT. 236 hyperfine transitions have been assigned for 47 rotational transitions of the $^{35}$Cl isotope of the GGT conformer, and 146 hyperfine and 37 rotational transitions were assigned to the $^{37}$Cl isotopomer. 128 hyperfine and 30 rotational transitions have also been assigned to the $^{35}$Cl isotope of the TGT conformation; 110 hyperfine and 28 rotational transitions were assigned to the $^{37}$Cl isotopomer. The extensive hyperfine splitting data, measured to high resolution with a mini FT microwave spectrometer, were used to determine both diagonal and off-diagonal elements of the $^{35}$Cl and $^{37}$Cl nuclear quadrupole coupling tensors. The experimental rotational constant data, as well as the $^{35}$Cl and $^{37}$Cl nuclear quadrupole coupling tensors, were compared to the results from 27 optimized ab initio (HF/6-311++G(d,p) and MP2/6-311++G(d,p)) model structures.