THE LABORATORY DETECTION AND GEOMETRICAL STRUCTURE OF THIOZONE (S_3) AND TETRASULFUR (S_4)

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Small sulfur clusters (S_2 – S_8) are of significant fundamental and applied interest, but surprisingly little is known about the electronic ground state and structures from S_3 to S_5. The rotational spectra of two, thiozone, S_3, and tetrasulfur, S_4, have now been observed for the first time by Fourier transform microwave spectroscopy. From the rotational constants of the normal and ^{34}S isotopic species, precise geometrical structures have been derived for both clusters with C_{2v} symmetry. The derived structural parameters indicate substantial double bonding in S_3 and sp^2 hybridization of the apex sulfur atom; S_4 also has double bonding between the outermost S atoms, but the central bond is relatively long and weak, like that observed for S_2O_2.