A LABORATORY AND THEORETICAL INVESTIGATION OF THE SILICON SULFUR MOLECULES H_2SiS AND Si_2S

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By means of Fourier transform microwave spectroscopy of a molecular beam, the rotational spectra of two small silicon sulfur molecules, the H_2SiS chain and the Si_2S ring, have been detected in the centimeter-wave band. Precise rotational and centrifugal distortion constants have been determined for both closed-shell species. Empirical equilibrium (r_e^{emp}) structures have been derived for both from the experimental rotational constants of the normal and rare isotopic species corrected for zero point vibrational effects through a quantum-chemical evaluation of the harmonic force fields. These structures compare very well with high-level theoretical structures obtained using the CCSD(T) method in combination with large basis sets up to cc-pwCVQZ. Because H_2SiS and Si_2S are closely-related in composition to the abundant astronomical molecule, SiS, and are calculated to be fairly polar, they are good candidates for radioastronomical detection in IRC+10216 and circumstellar shells of other evolved carbon stars.