

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

MICHAEL C. MCCARTHY and PATRICK THADDEUS, *Harvard-Smithsonian Center for Astrophysics, 60 Garden St., Cambridge, MA 02138, and School of Engineering & Applied Sciences, Harvard University, 29 Oxford St., Cambridge, MA 02138*; HARSHAL GUPTA, *Institute for Theoretical Chemistry, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, Texas 78712*; SVEN THORWIRTH, *Max-Planck-Institut für Radioastronomie, Auf dem Hügel 69, 53121 Bonn, Germany*; JÜRGEN GAUSS, *Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, Jakob-Welder-Weg 11, D-55128 Mainz, Germany*.

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.