

## FTMW SPECTROSCOPY OF SILYL MERCAPTAN, H<sub>3</sub>SiSH

S. THORWIRTH, *I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany*; V. LATTANZI, OSCAR MARTINEZ, JR., MICHAEL C. MCCARTHY, *Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, U.S.A. and School of Engineering and Applied Sciences, Harvard University, 29 Oxford Street, Cambridge, MA 02138, U.S.A.*; LI-HONG XU, *Department of Physics, Centre for Laser, Atomic and Molecular Studies (CLAMS) University of New Brunswick, Saint John, New Brunswick, Canada E2L 4L5.*

By means of Fourier transform microwave spectroscopy of a supersonic jet, the pure rotational spectrum of silyl mercaptan, H<sub>3</sub>SiSH, has been observed for the first time in a low-current dc discharge through a mixture of silane and hydrogen sulfide heavily diluted in neon. The spectroscopic identification was based on predictions from high-level quantum-chemical calculations at the CCSD(T) level of theory in combination with large basis sets performed using the CFOUR suite of programs<sup>a</sup>. In addition to the parent isotopic species, rotation lines of the rare isotopologs H<sub>3</sub><sup>29</sup>SiSH, H<sub>3</sub><sup>30</sup>SiSH, H<sub>3</sub>Si<sup>34</sup>SH, and D<sub>3</sub>SiSD have also been observed.

---

<sup>a</sup>CFOUR, Coupled-Cluster techniques for Computational Chemistry, a quantum-chemical program package by J.F. Stanton, J. Gauss, M.E. Harding, P.G. Szalay et al., for the current version, see <http://www.cfour.de>.