FTMW SPECTROSCOPY OF SILYL MERCAPTAN, H_3SiSH

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By means of Fourier transform microwave spectroscopy of a supersonic jet, the pure rotational spectrum of silyl mercaptan, H_3SiSH, 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[a]. In addition to the parent isotopic species, rotation lines of the rare isotopologs $H_3^{29}SiSH$, $H_3^{30}SiSH$, $H_3Si^{34}SH$, and D_3SiSD have also been observed.

[a]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.