ROTATIONAL SPECTRUM SPECTRUM AND COUPLED-CLUSTER CALCULATIONS OF SILICON OXYSULFIDE, O=Si=S

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Silicon oxysulfide, OSiS, and seven of its minor isotopic species have been characterized for the first time in the gas phase at high spectral resolution by means of Fourier-transform microwave spectroscopy. The equilibrium structure of OSiS has been determined from a combination of experimental ground state rotational constants and calculated vibrational corrections to those. The structural parameters are in good agreement with values from high-level quantum-chemical calculations using coupled-cluster techniques together with sophisticated additivity and extrapolation schemes.