

FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF THE HOSO RADICAL

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Molecules closely-related to SO₂ are of considerable interest because of the important role this triatomic or its surrogates play in the atmospheric and combustion chemistry of sulfur-containing compounds. Previous coupled-cluster quantum chemical calculations^a of the [HSO₂] potential energy surface conclude that a *cis*-isomer is the ground state, the *trans* isomer is a transition state, and that a C_{2v} HSO₂ isomer lies considerably higher in energy (~ 20 kcal/mol). Using Fourier Transform microwave spectroscopy, the rotational spectrum of the *cis*-HOSO radical has been precisely characterized for the first time by applying a DC discharge to a mixture of water and sulfur dioxide heavily diluted in neon. The fundamental rotational transition was detected near 17 GHz, in good agreement (within ~ 1%) of the calculated value derived from the equilibrium structure^b. Microwave-microwave double resonance techniques have been used to extend the dataset to higher frequencies and to provide confirmation of the spectroscopic assignments.

^aD. Binns, and P. Marshall, *Journal of Chemical Physics* **95**, 4940, (1991)

^bB. Napolion, and J. D. Watts, *Chemical Physics Letters* **421**, 562, (2006)