Fourier Transform Microwave Spectroscopy of the Hoso Radical

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Molecules closely-related to SO$_2$ 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 [HSO$_3$] potential energy surface conclude that a cis-isomer is the ground state, the trans isomer is a transition state, and that a $C_2v$ HSO$_3$ isomer lies considerably higher in energy ($\sim 20$ 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 $\sim 1\%$) 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.