BROADBAND AND CAVITY SPECTROSCOPY OF THIOFULMINIC ACID HCNS AND THIOISOFULMINIC ACID HSNC, AND A SYSTEMATIC ASTRONOMICAL SEARCH FOR THE FOUR [H,C,N,S] ISOMERS IN SGR B2 WITH THE GREEN BANK TELESCOPE

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The rotational spectra of thiofulminic acid, HCNS, and isothiofulminic acid, HSNC, two energetic [H,C,N,S] isomers calculated to lie about 35 kcal/mol above HNCS, have been observed at high spectral resolution by a combination of broadband and Fabry-Pérot FT microwave spectroscopy between 11 and 37 GHz. Searches for both isomers were based on high level coupled cluster calculations. Precise rotational, centrifugal distortion, and nitrogen hyperfine coupling constants have been determined for the normal and rare isotopic species of both closed-shell molecules; all in good agreement with theoretical predictions.

On the basis of this work and prior rotational spectroscopy on HNCS and HSCN, a systematic search for the four [H,C,N,S] isomers has been undertaken towards Sgr B2 using the 100 m Green Bank Telescope. In Sgr B2(M), we find no evidence for either HCNS or HSNC, and surprisingly no evidence for the ground state HNCS, but there is very suggestive evidence for HSCN, the second most stable isomer calculated to lie approximately 6 kcal/mol higher in energy.[a] A summary of our observations towards Sgr B2(M) and other regions of Sgr B2 will be presented.