

MICROWAVE SPECTROSCOPIC AND THEORETICAL EXAMINATION OF ALLYL ISOTHIOCYANATE CONFORMATIONAL SPACE

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A spectroscopic analysis of allyl isothiocyanate ($\text{CH}_2 = \text{CHCH}_2\text{NCS}$) was conducted via chirped-pulse and Balle-Flygare Fourier Transform microwave (FTMW) spectroscopy in the 7-25 GHz range. Rotational transitions associated with the different conformers were assigned based on information gathered from quantum-chemical calculations computed at B3LYP-D3(BJ) and MP2 levels of theory using the Dunning cc-pVTZ basis set. The results showed the existence of two conformers, the gauche conformer, which was reported in previous work^a as well as the first reported existence of a second conformer which corresponds to the global minimum. Spectroscopic assignments included transitions due to both parent conformers, ³⁴S, ¹³C and ¹⁵N singly substituted isotopic species as well as hyperfine splitting due to the presence of ¹⁴N.

^aMaiti, S.; Jaman, A. I.; Nandi, R. N. *J. Mol. Spectrosc.* **165** (1994), 168-172