

## EXPLORING THE PROPERTIES AND REACTIVITY OF CARBONYL DIISOTHIOCYANATE WITH ROTATIONAL SPECTROSCOPY

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Accessing simple molecules is crucial to our understanding of chemical reactivity. Particularly, characterization of heavier homologues of molecules essential to life, *e.g.*, carbonic acid and urea, can lead to new insights. Synthetic routes to such compounds, followed by exploration of their reactivity, could not only deepen our knowledge of synthetic chemistry, but also create the basis for novel applications and new research fields. It is known that the reactivity and properties of a compound are a function of its structure. Subsequently, exploring molecular structure in an isolated environment in the absence of lattice and solvent effects is key to our understanding of the structure vs properties relationship.

Carbonyl diisothiocyanate (CDIT),  $C_3N_2O_2S_2$ , a highly unstable and reactive compound, was first synthesized in 1902.<sup>1</sup> It recently has been characterized in the condensed phase,<sup>2</sup> however, to the best of our knowledge, this is the first study addressing its properties in the gas phase. The rotational spectra of two isomers of CDIT, *syn-syn* and *syn-anti*, were recorded with Chirped Pulse Fourier Transform Microwave (CP-FTMW). Presence of two quadrupolar nuclei ( $N, I=1$ ) results in hyperfine splitting of rotational transitions, which is analyzed and provides a direct insight into the electronic environment of the molecule. Detection of  $^{13}C$ ,  $^{34}S$ ,  $^{15}N$  and  $^{18}O$  isotopologues in their natural isotopic abundances allowed for structure determination of the most abundant *syn-syn* isomer in the gas phase. The gas phase structure is compared to the previously determined crystal structure and demonstrates a high level of consistency. Spectral analysis is guided by quantum chemical calculations and CDIT, owing to the isothiocyanate substituents, makes an interesting case for theoretical benchmarking.

<sup>1</sup> Dixon, A. E., *Proc. Chem. Soc., London*, 1902, 18 (257), 235

<sup>2</sup> Pfeiffer, J.; Trost, C.; Pachkovska, A.; and Tambornino, F.; *Inorg. Chem*, 2021, 60 (14) 10722–10728