

MILLIMETER-WAVE SPECTROSCOPY OF FORMYL AZIDE (HC(O)N₃)

NICHOLAS A. WALTERS, BRENT K. AMBERGER, BRIAN J. ESSELMAN, R. CLAUDE WOODS,
ROBERT J. McMAHON, *Department of Chemistry, University of Wisconsin, Madison, WI, USA.*

Formyl azide (HC(O)N₃) is a highly unstable molecule ($t_{1/2} \sim 2$ hours at room temperature as a gas) that has only recently been studied spectroscopically by UV, IR, Raman and NMR methods.^{ab} We have synthesized formyl azide and obtained its absorption spectrum at room temperature over the range 250-360 GHz. As in the case of carbonyl diazide,^c two conformers are expected for HC(O)N₃, with the *syn*-isomer 2.8 kcal/mol lower in energy than the *anti*-isomer (CCSD(T)/ANO1). Calculations at the same level of theory and the same basis set predict the dipole moments for the *syn*-isomer ($\mu = 1.56$ D) and *anti*-isomer ($\mu = 2.56$ D). These calculations also indicate that *b*-type transitions should dominate the *syn*-isomer spectrum, while *a*-type transitions become more significant in the case of the *anti*-isomer. Despite the *anti*-isomer having a larger dipole moment, the *syn*-isomer still gives rise to all the dominant features of the spectrum. Thus far, five vibrational states (ν_9 , ν_{12} , $2\nu_9$, $\nu_9 + \nu_{12}$, ν_{11}) have been studied for the *syn*-isomer, with the highest energy state $\nu_{11} = 582.6$ cm⁻¹. Searches for the spectra of the *anti*-isomer are ongoing.

^aBanert, K. et al. *Angew. Chem. Int. Ed.* **2012**, 51, 4718-4721

^bZeng, X. et al. *Angew. Chem. Int. Ed.* **2013**, 52, 3503-3506

^cAmberger, B.K. et al. *J. Mol. Spectrosc.* **259**, (2014) 15-20