

SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE OF 1H- AND 2H-1,2,3-TRIAZOLES (C₂H₃N₃)

MARIA ZDANOVSKAIA, BRIAN J. ESSELMAN, SAMUEL M. KOUGIAS, *Department of Chemistry, University of Wisconsin-Madison, Madison, WI, USA*; JOHN F. STANTON, *Quantum Theory Project, University of Florida, Gainesville, FL, USA*; R. CLAUDE WOODS, ROBERT J. McMAHON, *Department of Chemistry, University of Wisconsin-Madison, Madison, WI, USA*.

1H-1,2,3-triazole (C_s; $\kappa = 0.94$; $\mu_a = 4.1$ D, $\mu_b = 1.6$ D) and 2H-1,2,3-triazole (C_{2v}; $\kappa = 0.82$; $\mu_b = 0.52$ D) are tautomers (C₂H₃N₃), the former of which is formally the product of a 1,3-dipolar cycloaddition of two explosive compounds, hydrazoic acid and acetylene. We have analyzed the rotational spectra of these tautomers in the 130 – 360 GHz frequency range and least-squares fit the observed transitions to sextic Hamiltonians with low error ($\sigma < 50$ kHz). While ¹³C and ¹⁵N isotopologues have been observed at natural abundance and similarly analyzed, several synthetic techniques had to be employed to access deuterium-substituted isotopologues. The rotational constants of the numerous isotopologues, along with vibration-rotation interaction and electron mass corrections predicted using coupled-cluster and density functional theories, have been used to determine highly precise semi-experimental equilibrium structures (r_e^{SE}) of the 1,2,3-triazoles. Equilibrium structures calculated at the above-mentioned levels of theory, as well as a computational prediction using basis set extrapolation and additional corrections for the 2H structure, are compared to the semi-experimental structures.