

## SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE OF 1H- AND 2H-1,2,3-TRIAZOLES (C<sub>2</sub>H<sub>3</sub>N<sub>3</sub>)

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1H-1,2,3-triazole (C<sub>s</sub>;  $\kappa = 0.94$ ;  $\mu_a = 4.1$  D,  $\mu_b = 1.6$  D) and 2H-1,2,3-triazole (C<sub>2v</sub>;  $\kappa = 0.82$ ;  $\mu_b = 0.52$  D) are tautomers (C<sub>2</sub>H<sub>3</sub>N<sub>3</sub>), 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 <sup>13</sup>C and <sup>15</sup>N 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.