IMPROVED SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE DETERMINATION AND THEORETICAL PREDICTION OF HYDRAZOIC ACID (HN_3)

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We conducted multiple high-level *ab initio* calculations to obtain improved semi-experimental equilibrium structures (${r_e}^{SE}$) of hydrazoic acid (HN_3) using previously reported experimental data and to obtain improved, purely theoretical predictions of the structure. For the ${r_e}^{SE}$ structures, we used the isotopologue-dependent vibrational corrections to the ground rotational constants obtained from anharmonic VPT2 calculations at CCSD(T) using cc-pVXZ and cc-pCVXZ basis sets (where $X = D, T, Q, 5$), as well as the isotopologue-dependent electron-mass corrections at the same level of theory, to carry out nonlinear least-squares fits of the experimentally determined rotational constants for all but two of the HN_3 isotopologues. The extent of corrections that were calculated allowed for extrapolation of the ${r_e}^{SE}$ structure to the complete basis set limit. To achieve an improved theoretical prediction, we obtained a CCSD(T)/cc-pCV6Z optimization and included corrections for extrapolation to the complete basis set limit, for effects of electron correlation, for relativistic effects, and for the Born-Oppenheimer approximation. The parameters of the resulting theoretical structure agrees to within the 2σ uncertainties of the ${r_e}^{SE}$.