SPECTROSCOPIC CHARACTERIZATION OF HIGHLY ENERGETIC ISOFULMINIC ACID, HONC, BY EXPERIMENTAL AND THEORETICAL APPROACHES

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The highly energetic isomer isofulminic acid, HONC, calculated to lie more than 80 kcal/mol above HNCO[a], has been characterized spectroscopically in its ground state by a combination of rotational spectroscopy and large-scale CCSD(T) electronic structure calculations. The fundamental rotational transition of HONC, $H^{18}ONC$, $HON^{13}C$, and DONC has been detected in the centimeter-wave band in a molecular beam by Fourier transform microwave spectroscopy, and effective rotational constants and nitrogen and deuterium quadrupole coupling constants have been derived for each isotopic species. All of the measured constants agree very well with those predicted from theoretical calculations of HONC. A number of other electronic and spectroscopic properties of isofulminic acid, including dipole moments, vibrational frequencies, and infrared intensities have also been calculated at the CCSD(T)/cc-pCVQZ level of theory. HONC is a good candidate for detection in space with radio telescopes because of its high polarity and because the more stable isomers, HNCO, HOCN, and HCNO have been identified in rich astronomical sources.

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