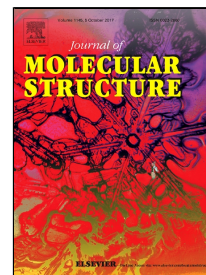


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# Structure, Thermodynamic and Electronic Properties of Carbon-Nitrogen Cubanes and Protonated Polynitrogen Cations

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**Abstract.** Energy generation and storage are at the center of modern civilization. Energetic materials constitute quite a large class of compounds with a high amount of stored chemical energy that can be released. We hereby use a combination of quantum chemistry methods to investigate feasibility and properties of carbon-nitrogen cubanes and multi-charged polynitrogen cations in the context of their synthesis and application as unprecedented energetic materials. We show that the stored energy increases gradually with the nitrogen content increase. Nitrogen-poor cubanes retain their stabilities in vacuum, even at elevated temperatures. Such molecules will be probably synthesized at some point. In turn, polynitrogen cations are highly unstable, except  $N_8H^+$ , despite they are isoelectronic to all-carbon cubane. Kinetic stability of the cation decays drastically as its total charge increases. High-level thermodynamic calculations revealed that large amounts of energy are liberated upon decompositions of polynitrogen cations, which produce molecular nitrogen, acetylene, and protons. The present results bring a substantial insights to the design of novel high-energy compounds.

**Key words:** cubane; stability; thermodynamics; molecular dynamics; PM7-MD.

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