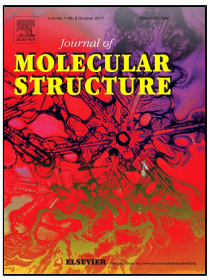
Accepted Manuscript



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

Vitaly V. Chaban, Nadezhda A. Andreeva

PII:	S0022-2860(17)31130-4
DOI:	10.1016/j.molstruc.2017.08.063
Reference:	MOLSTR 24201
To appear in:	*Journal of Molecular Structure*
Received Date:	29 July 2017
Revised Date:	16 August 2017
Accepted Date:	16 August 2017

Please cite this article as: Vitaly V. Chaban, Nadezhda A. Andreeva, Structure, Thermodynamic and Electronic Properties of Carbon-Nitrogen Cubanes and Protonated Polynitrogen Cations, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc.2017.08.063

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

Vitaly V. Chaban[1] and Nadezhda A. Andreeva[2]

1) P.E.S., Vasilievsky Island, Saint Petersburg, Leningrad oblast, Russian Federation.
2) PRAMO, St Petersburg, Leningrad oblast, Russian Federation.

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 N8H+, 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.