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Title:	Aromaticity and hydrogen storage capability of planar N6 4-and N4 2 rings.
Authors:	Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	AIN Aromaticities Counter cations Induced magnetic fields
Issue Date:	2011
Publisher:	Elsevier B.V.
Citation:	Chemical Physics Letters, 506 (4-6), pp. 315-320.
Abstract:	Theoretical investigation on planar N64- and N42- rings has been performed. The aromaticity of the rings has been analyzed through their nucleus independent chemical shift (NICS) values as well as the σ - and π -contribution of the Z-component of the induced magnetic field. Counter to a previously reported result [Chem. Phys. Lett. 432 (2006) 331], the N6 4- ring is found to be a local minimum and aromatic with planar D6h symmetry. The N6 2- ring exhibits conflicting aromaticity like AIN44-. Both the N64- and N42- rings can be stabilized in presence of suitable counter cations and systems like N 6Ca2 and N4Li2 can trap molecular hydrogen.
Description:	Only IISERM authors are available in the record.
URI:	http://www.sciencedirect.com/science/article/pii/S000926141100306X (http://www.sciencedirect.com/science/article/pii/S000926141100306X) http://dx.doi.org/10.1016/j.cplett.2011.03.037 (http://dx.doi.org/10.1016/j.cplett.2011.03.037)
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