Title:	Design, Synthesis, and Structural Analysis of Divalent NI Compounds and Identification of a New Electron-Donating Ligand
Authors:	Khullar, S. (/jspui/browse?type=author&value=Khullar%2C+S.) Gupta, Vijay (/jspui/browse?type=author&value=Gupta%2C+Vijay) Mandal, S.K. (/jspui/browse?type=author&value=Mandal%2C+S.K.)
Keywords:	Carbene ligands Density functional calculations Ligand design Nitrogen
Issue Date:	2016
Publisher:	Wiley-VCH Verlag
Citation:	Chemistry - A European Journal, 22(3), pp. 1088-1096
Abstract:	The dative-bond representation (L→E) in compounds with main group elements (E) has triggered extensive debate in the recent past. The scope and limits of this nonclassical coordination bond warrant comprehensive exploration. Particularly compounds with (L→N←L′)+ arrangement are of special interest because of their therapeutic importance. This work reports the design and synthesis of novel chemical species with the general structural formula (L→N←L′)+ carrying the unusual ligand cyclohexa-2,5-diene-4-(diaminomethynyl)-1-ylidene. Four species belonging to the (L→N←L′)+ class carrying this unconventional ligand were synthesized. Quantum chemical and X-ray diffraction analyses showed that the electronic and geometric parameters are consistent with those of already reported divalent NI compounds. The molecular orbital analysis, geometric parameters, and spectral data clearly support the L→N and N←L′ interactions in these species. The newly identified ligand has the properties of a reactive carbene and high nucleophilicity.
Description:	Only IISERM authors are available in the record.
URI:	https://chemistry-europe.onlinelibrary.wiley.com/doi/full/10.1002/chem.201503618 (https://chemistry-europe.onlinelibrary.wiley.com/doi/full/10.1002/chem.201503618) http://hdl.handle.net/123456789/2498 (http://hdl.handle.net/123456789/2498)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/2498/1/Need%20to%20add%20pdf.odt)		7.9 kB	OpenDocument Text	View/Open (/jspui/bitstream/12345

Show full item record (/jspui/handle/123456789/2498?mode=full)
(/jspui/handle/123456789/2498/statistics)