Dimeric nature of N-coordinated Mg and Ca ions in metaloorganic compounds. The topological analysis of ELF functions for Mg—Mg and Ca—Ca bonds.

Autorzy

Sławomir Berski

Piotr Durlak

Rok wydania

2017

Czasopismo

Polyhedron

Numer woluminu

129

Strony

22-29

DOI

10.1016/j.poly.2017.03.024

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The local electronic structure of the Mg–Mg and Ca–Ca bonds have been investigated in the modeldimeric magnesium(I) and calcium(I) molecules: [C10H18Mg2N4], and [C10H18Ca2N4] using the topolog-ical analysis of Electron Localisation Function (ELF). The wave function has been approximated by theDFT method and PBE, B3LYP, M052X, M062X,xB97XD, CAM-B3LYP, LC-xPBE and B2PLYP functionals.The investigated bonds are covalent, and are represented by disynaptic bonding attractors V(Mg,Mg)and V(Ca,Ca). The basin population of the Ca–Ca bond (1.84–1.89e) is about 0.1e smaller than popula-tion of the Mg–Mg bond (1.95–1.98e). The results of ELF-analysis support classical Lewis representationof the 2c–2e bonds (single bond). The topological analysis of electron density field,q(r) shows that boththe Mg–Mg and Ca–Ca bonds are characterised by the non-nuclear attractor (NNA) and pseudo-basinlocalised in midpoint of the bond. However, in the case of the Ca–Ca bond its localisation dependson the used functional. The median ELF-basin population of the Mg–Mg bond (1.96e) is about 2.5 largerthan the population (0.79e) of pseudo-atomic basin associated with NNA of theq(r) field. The analysisperformed for the nitrogen – magnesium and nitrogen–calcium bonds showed the dative bonds N?Mgand N?Ca with very large values of the polarity index, pNMg,pNCa, 0.96 and median ELF-basin popu-lation 3.40e.

Słowa kluczowe

Magnesium(I) and Calcium(I) compounds, Electron localization function (ELF), Topological analysis, atoms in molecules, Attractor and Chemical bond