

Static and Dynamical Quantum Studies of CX_3-AlX_2 and $CSiX_3-BX_2$ ($X = F, Cl, Br$) Complexes with Hydrocyanic Acid: Unusual Behavior of Strong π -Hole at Triel Center

Autorzy

Mariusz Michalczyk

Kamil Wojtkowiak

Jarosław J. Panek

Aneta Jezierska

Wiktor Zierkiewicz

Rok wydania

2023

Czasopismo

International Journal of
Molecular Sciences

Numer woluminu

24

Strony

7881/1-7881/20

DOI

10.3390/ijms24097881

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The set of TX_3-TrX_2 ($T = C, Si, Ge$; $Tr = B, Al, Ga$; $X = F, Cl, Br$) molecules offers a rather unique opportunity to study both σ -hole and π -hole dimerization on the tetrel and triel ends, respectively. According to the molecular electrostatic potential (MEP) distribution, the π -hole extrema (acidic sites) were more intense than their σ -hole counterparts. The molecules owning the most (CX_3-AlX_2) and least (SiX_3-BX_2) intense π -holes were chosen to evaluate their capacities to attract one and two HCN molecules (Lewis bases). We discovered that the energetic characteristics of π -hole dimers severely conflict with the monomers MEP pattern since the weakest π -hole monomer forms a dimer characterized by interaction energy compared to those created by the monomers with noticeably greater power in the π -hole region. This outcome is due to the deformation of the weakest π -hole donor. Furthermore, the MEP analysis for monomers in the geometry of respective dimers revealed a “residual π -hole” site that was able to drive second ligand attachment, giving rise to the two “unusual trimers” examined further by the NCI and QTAIM analyses. Apart from them, the π -hole/ π -hole and σ -hole/ π -hole trimers have also been obtained throughout this study and described using energetic and geometric parameters. The SAPT approach revealed details of the bonding in one of the “unusual trimers”. Finally, Born-Oppenheimer Molecular Dynamics (BOMD) simulations were carried out to investigate the time evolution of the interatomic distances of the studied complexes as well as their stability.

Słowa kluczowe

molecular electrostatic potential, triel bond, QTAIM, NCI, SAPT, BOMD

Licencja otwartego dostępu

CC-BY

Licencja na prawach której można swobodnie kopiować, rozprowadzać, zmieniać i remiksować objęty prawem autorskim utwór (Utwór-przedmiot prawa autorskiego) pod warunkiem podania imienia i nazwiska autora utworu pierwotnego oraz źródła pochodzenia utworu.

Pełny tekst licencji:

<https://creativecommons.org/licenses/by/3.0/pl/legalcode>

Adres publiczny

<http://dx.doi.org/10.3390/ijms24097881>

Strona internetowa wydawcy

<http://www.mdpi.com/journal/metals>