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Research Article

Competition between σ -hole pnictogen bond and π -hole tetrel bond in complexes of $\text{CF}_2=\text{CFZH}_2$ ($\text{Z} = \text{P}, \text{As}, \text{and Sb}$)

Wenbo Dong, Yu Wang, Jianbo Cheng, Xin Yang & Qingzhong Li

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ABSTRACT

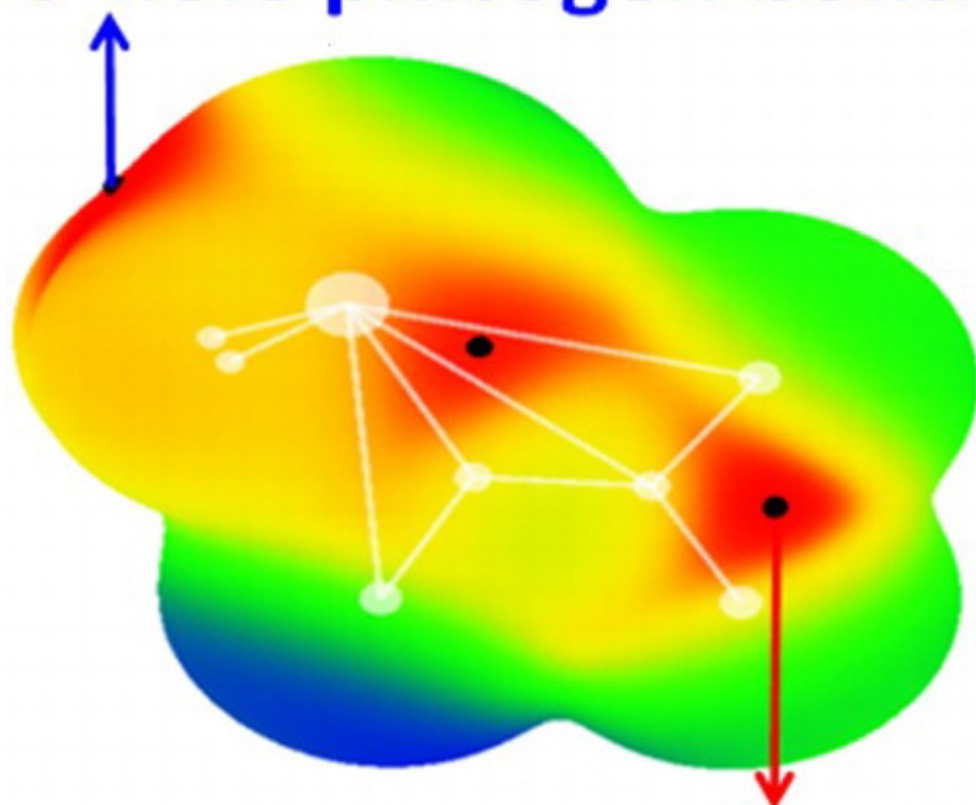
A computational study of the complexes formed by $\text{F}_2\text{C}=\text{CFZH}_2$ ($\text{Z} = \text{P}, \text{As}, \text{and Sb}$) and $\text{F}_2\text{C}=\text{CFPF}_2$ with two Lewis bases (NH_3 and NMe_3) has been carried out. In general, two minima complexes are found, one with a σ -hole pnictogen bond and the other one with a π -hole tetrel bond in most complexes but two σ -hole pnictogen bonded complexes are obtained for $\text{F}_2\text{C}=\text{CFZH}_2$ and NH_3 . They have similar stability though $\text{F}_2\text{C}=\text{CFSbH}_2$ engages in a much stronger σ -hole pnictogen bond with NMe_3 . The $-\text{PF}_2$ substitution makes the π -hole on the terminal carbon form a tetrel bond with NH_3 . A heavier $-\text{ZH}_2$ group engages in a stronger σ -hole pnictogen bond but results in a weaker π -hole tetrel bond. Other than electrostatic interaction, the stability of both complexes is attributed

to the charge transfer from the N lone pair into the C-Z/H-Z anti-bonding orbital in the pnictogen bond and the C=C anti-bonding orbital in the tetrel bond.

The σ -hole pnictogen bonded and π -hole tetrel bonded complexes between $F_2C=CFZH_2$ ($Z = P, As, \text{ and } Sb$) and two Lewis bases (NH_3 and NMe_3) have been compared. The results indicate that both interactions can compete, dependent on the nature of the N base.

GRAPHICAL ABSTRACT

σ -hole pnictogen bond



π -hole tetrel bond

KEYWORDS:

σ -hole pnictogen bond

π -hole tetrel bond

NBO

AIM

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Additional information

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Related Research Data

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Binding Mechanisms in Supramolecular Complexes

Source: Angewandte Chemie International Edition

Characterizing the interplay of Pauli repulsion, electrostatics, dispersion and charge transfer in halogen bonding with energy decomposition analysis

Source: Physical Chemistry Chemical Physics

VMD: Visual molecular dynamics

Source: Journal of Molecular Graphics

Competition and cooperativity between tetrel bond and chalcogen bond in complexes involving F2CX (X = Se and Te)

Source: Chemical Physics Letters

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