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Research Article

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

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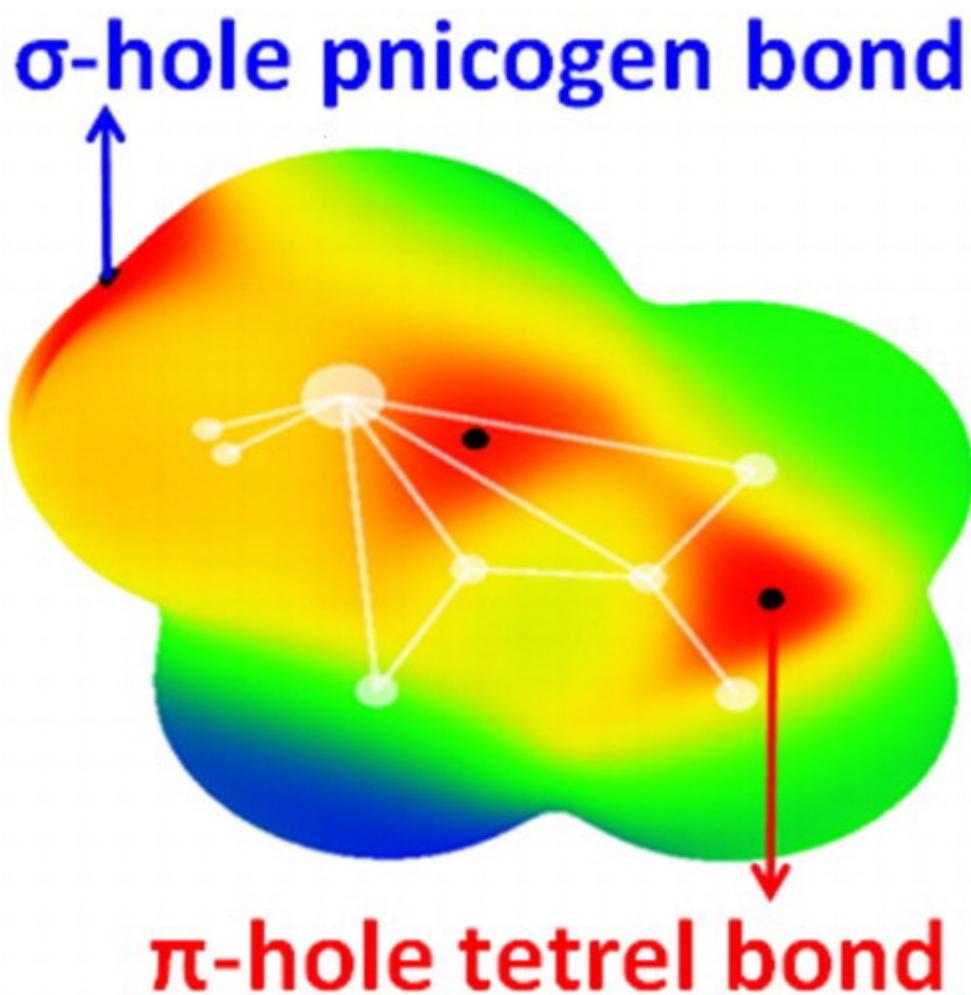
ABSTRACT

A computational study of the complexes formed by $\text{F}_2\text{C}=\text{CFZH}_2$ (Z = P, As, 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 pnicogen bond and the other one with a π -hole tetrel bond in most complexes but two σ -hole pnicogen 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 pnicogen 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 pnicogen 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 pnicogen bond and the C=C anti-bonding orbital in the tetrel bond.

The σ -hole pnicogen bonded and π -hole tetrel bonded complexes between $\text{F}_2\text{C}=\text{CFZH}_2$ ($\text{Z} = \text{P, As, and Sb}$) 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



KEYWORDS:

σ -hole pnicogen bond

π -hole tetrel bond

NBO

AIM

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Additional information

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