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Research Article

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

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

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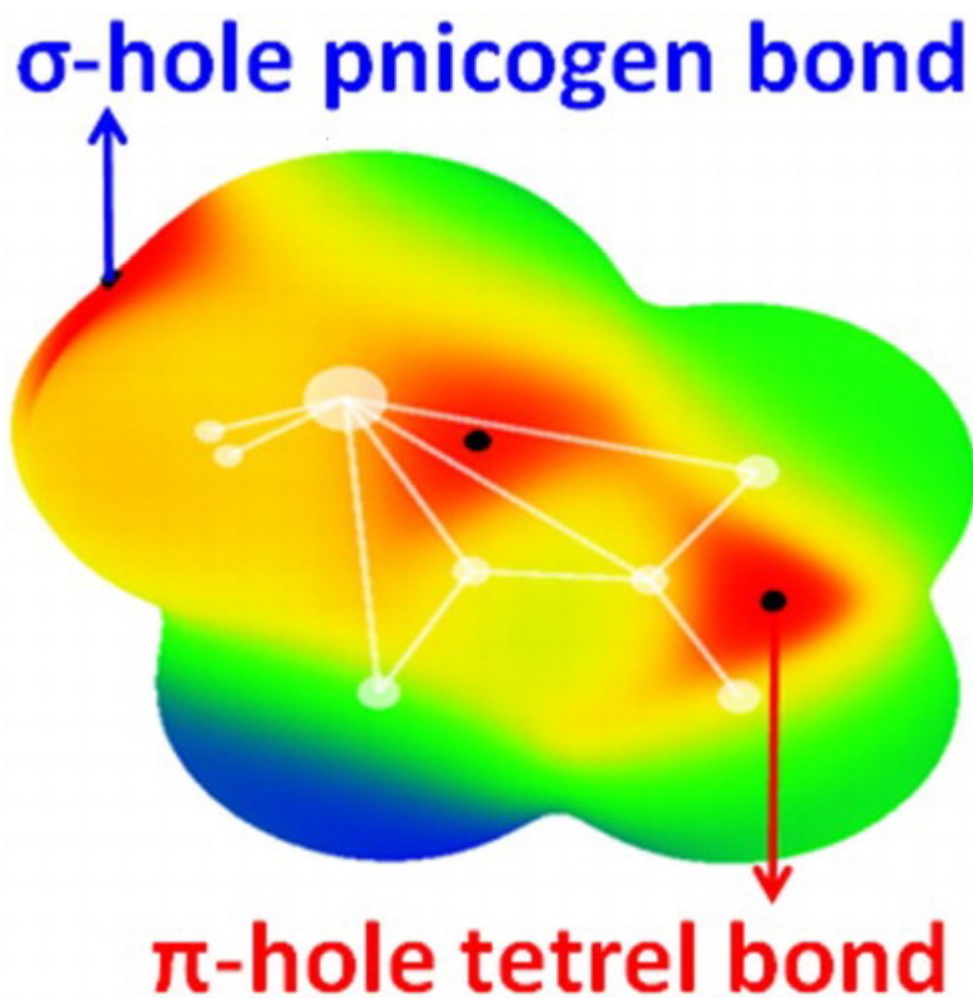
## ABSTRACT

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 ( $\text{NH}_3$  and  $\text{NMe}_3$ ) has been carried out. In general, two minima complexes are found, one with a  $\sigma$ -hole pnictogen bond and the other one with a  $\pi$ -hole tetrel bond in most complexes but two  $\sigma$ -hole pnictogen bonded complexes are obtained for  $\text{F}_2\text{C}=\text{CFZH}_2$  and  $\text{NH}_3$ . They have similar stability though  $\text{F}_2\text{C}=\text{CFSbH}_2$  engages in a much stronger  $\sigma$ -hole pnictogen bond with  $\text{NMe}_3$ . The  $-\text{PF}_2$  substitution makes the  $\pi$ -hole on the terminal carbon form a tetrel bond with  $\text{NH}_3$ . A heavier  $-\text{ZH}_2$  group engages in a stronger  $\sigma$ -hole pnictogen bond but results in a weaker  $\pi$ -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  $\sigma$ -hole pnictogen bonded and  $\pi$ -hole tetrel bonded complexes between  $F_2C=CFZH_2$  (Z = 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:

$\sigma$ -hole pnictogen bond

$\pi$ -hole tetrel bond

NBO

AIM

## Disclosure statement

No potential conflict of interest was reported by the authors.

# Additional information

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