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Research Article

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

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## ABSTRACT

A computational study of the complexes formed by  $\text{F}_2\text{C}=\text{CFZH}_2$  ( $Z = \text{P, As, and Sb}$ ) and

$\text{F}_2\text{C}=\text{CFH}_2$  and  $\text{F}_2\text{C}=\text{CFZ}_2$  (Z = P, As, and Sb) complexes are obtained. The  $\sigma$ -hole tetrel bond. Other complexes are attributed to the chalcogen orbital in the  $\text{F}_2\text{C}=\text{CFZH}_2$  (Z = P, As, and Sb) and two Lewis bases ( $\text{NH}_3$  and  $\text{NMe}_3$ ) have been compared. The

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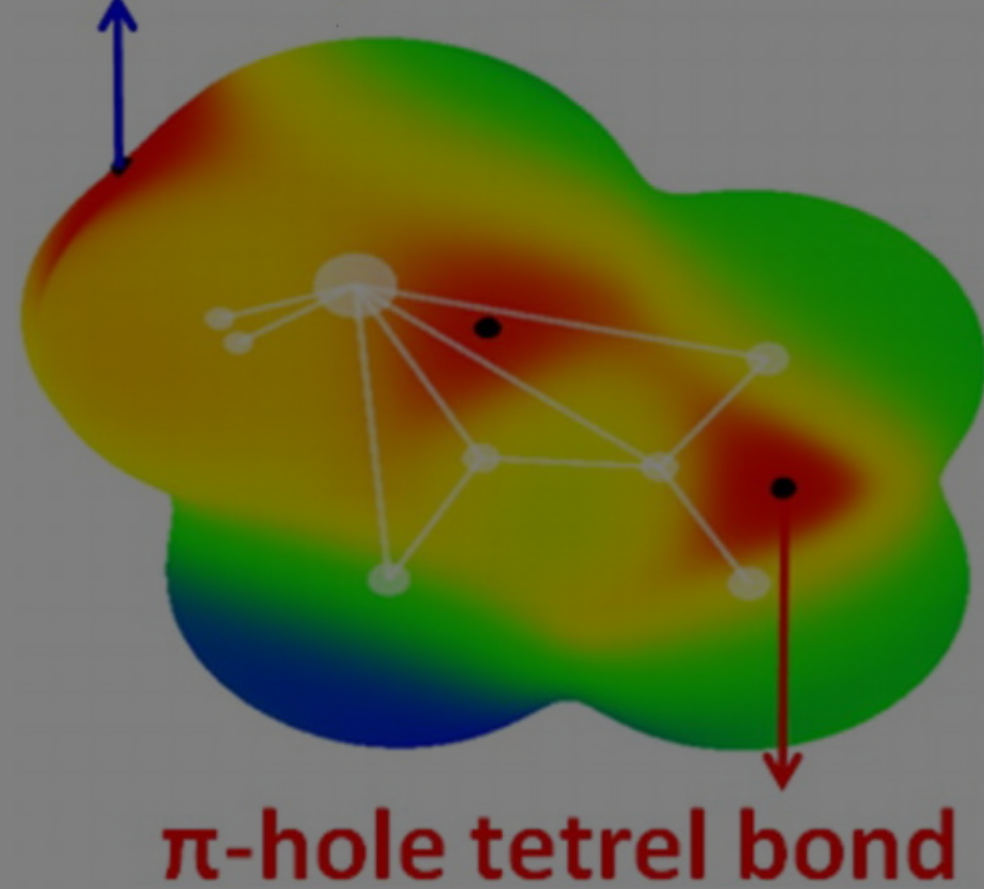
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results indicate that both interactions can compete, dependent on the nature of the N base.

GRAPHICAL ABSTRACT

# $\sigma$ -hole pnictogen bond



# $\pi$ -hole tetrel bond

KEYWORDS:  $\sigma$ -hole pnictogen bond  $\pi$ -hole tetrel bond NBO AIM

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

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