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Research Article

Competition between σ -hole pnicogen bond and π -hole tetrel bond in complexes of $CF_2 = CFZH_2$ (Z = P, As, and Sb)

Wenbo Dong, Yu Wang, Jianbo Cheng, Xin Yang & Qingzhong Li Pages 251-259 | Received 12 Jun 2018, Accepted 24 Jul 2018, Published online: 12 Aug 2018

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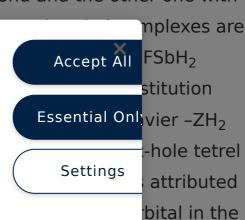
ABSTRACT

A computational study of the complexes formed by $F_2C=CFZH_2$ (Z = P, As, and Sb) and F₂C=CFPF₂ with two Lewis bases (NH₃ and NMe₃) 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 obtained engages makes grou bond. to the cl pnicoge

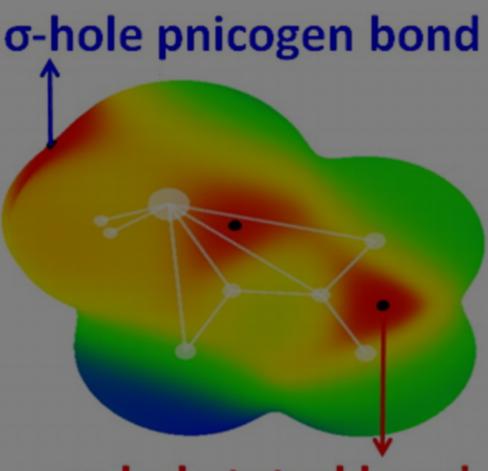
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The σ -hole pnicogen bonded and π -hole tetrel bonded complexes between $F_2C=CFZH_2$ (Z = P, As, and Sb) and two Lewis bases $(NH_3 \text{ and } NMe_3)$ have been compared. The results indicate that both interactions can compete, dependent on the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

GRAPHICAL ABSTRACT



π-hole tetrel bond

Q KEYWORDS: σ -hole pnicogen bond π -hole tetrel bond NBO AIM

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