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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

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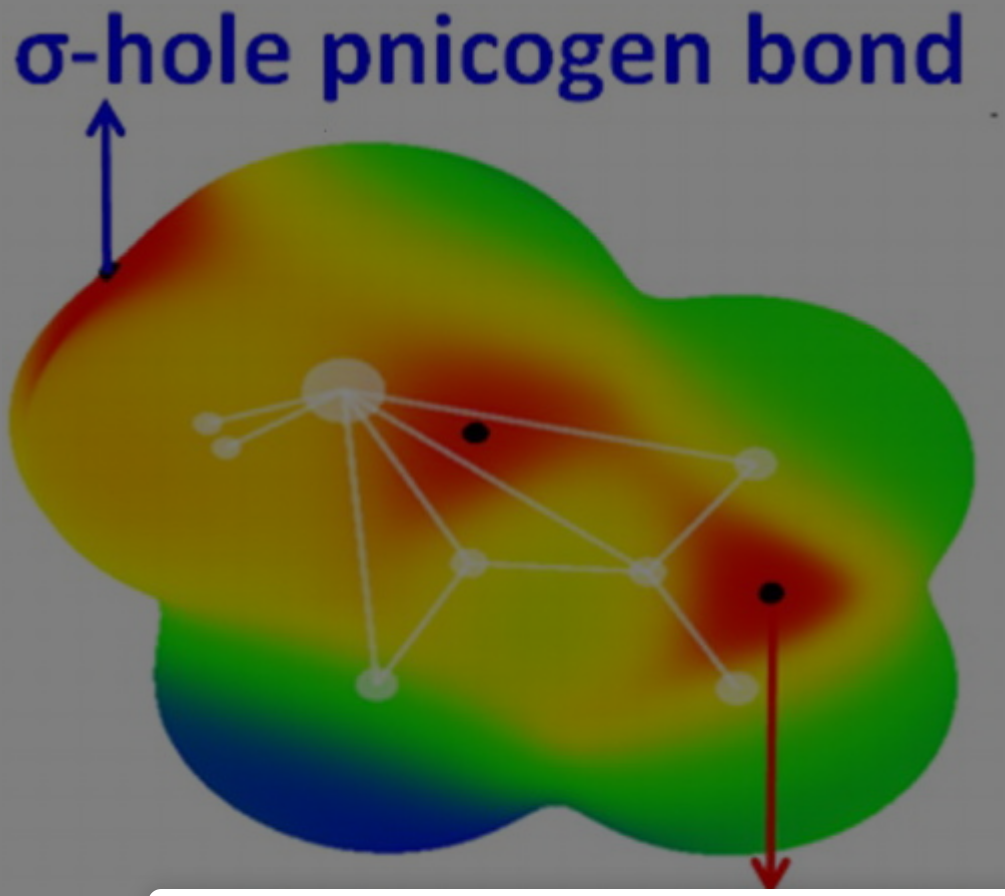
ABSTR...

A compu... nd Sb) and F_2C=CFP... eneral, two minima... er one with a π-h... mplexes are obtained... $FSbH_2$ engages... stitution makes t... vier –ZH_2 group er... -hole tetrel bond. Ot... attributed to the ch... bital 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 $F_2C{=}CFZH_2$ (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



KEYWORI

σ-hole pni

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σ-holes and π-holes: Similarities and differences
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The cooperativity between the σ-hole and π-hole interactions in the ClO···XONO2/XONO···NH3 (X = Cl, Br, I) complexes
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Source: Journal of Fluorine Chemistry
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