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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)

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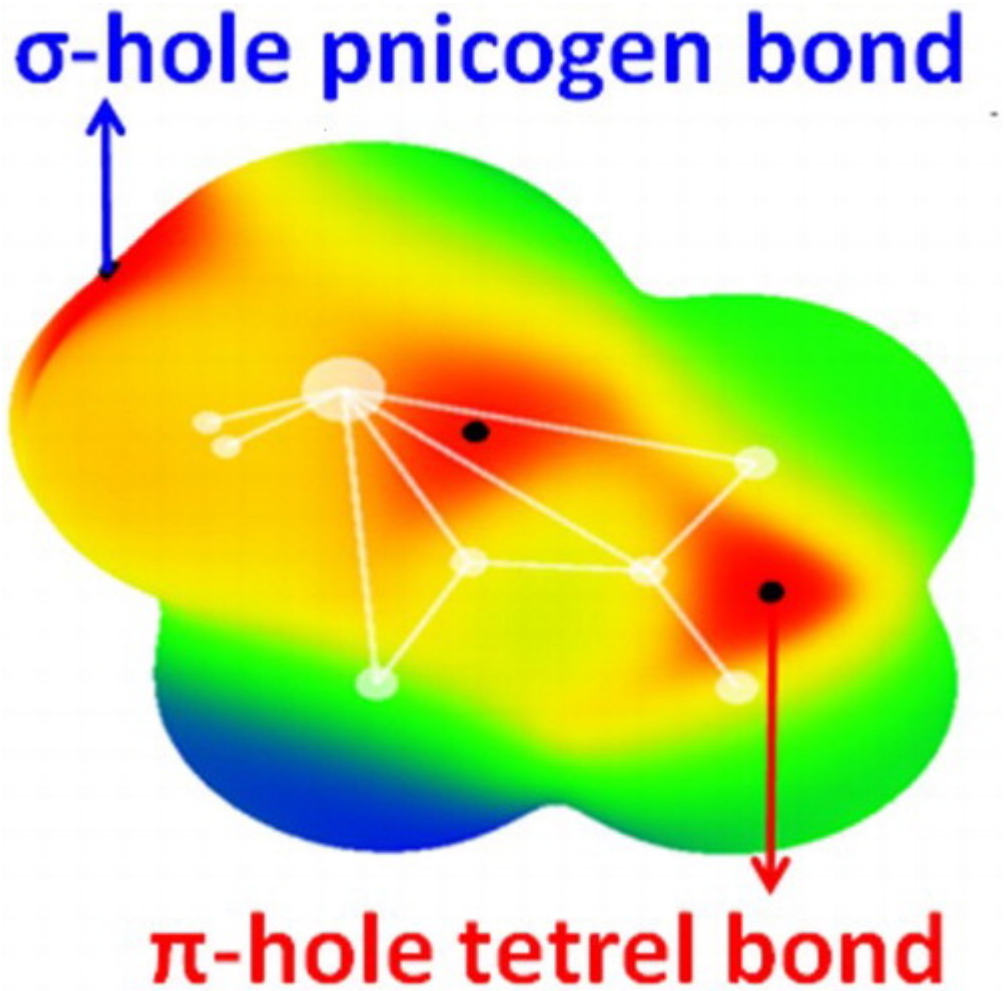
ABSTRACT

A computational study of the complexes formed by F_2C=$CFZH_2$ (Z = P, As, and Sb) and F_2C=$CFPF_2$ 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 F_2C=$CFZH_2$ and NH_3. They have similar stability though F_2C=$CFSbH_2$ engages in a much stronger σ-hole pnicogen bond with NMe_3. The $-PF_2$ substitution makes the π-hole on the terminal carbon form a tetrel bond with NH_3. A heavier $-ZH_2$ 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 $F_2C{=}CFZH_2$ (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:

σ-hole pnicogen bond | π-hole tetrel bond | NBO | AIM

Disclosure statement

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Additional information

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Source: Physical Chemistry Chemical Physics
VMD: Visual molecular dynamics
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