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Research Article
Competition between $\sigma$-hole pnicogen bond and $\pi$-hole tetrel bond in complexes of $\mathrm{CF}_{2}=\mathrm{CFZH}_{2}(\mathrm{Z}=\mathrm{P}, \mathrm{As}$, and Sb$)$
Wenbo Dong, Yu Wang, Jianbo Cheng, Xin Yang \& Qingzhong Li $\sim$
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## ABSTRACT

A computational study of the complexes formed by $\mathrm{F}_{2} \mathrm{C}=\mathrm{CFZH} \mathrm{C}_{2}(\mathrm{Z}=\mathrm{P}, \mathrm{As}$, and Sb ) and $\mathrm{F}_{2} \mathrm{C}=\mathrm{CFPF}_{2}$ with two Lewis bases $\left(\mathrm{NH}_{3}\right.$ and $\left.\mathrm{NMe}_{3}\right)$ has been carried out. In general, two minima complexes are found, one with a $\sigma$-hole pnicogen bond and the other one with a $\pi$-hole obtainec engages makest grou bond. to the cr

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( $\mathrm{Z}=\mathrm{P}, \mathrm{As}$, and Sb ) and two Lewis bases $\left(\mathrm{NH}_{3}\right.$ and $\left.\mathrm{NMe}_{3}\right)$ have been compared. The
results indicate that both interactions can compete, dependent on the nature of the N
base.
GRAPHICAL ABSTRACT


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The $\sigma$-hole pnicogen bonded and $\pi$-hole tetrel bonded complexes between $\mathrm{F}_{2} \mathrm{C}=\mathrm{CFZH} \mathrm{C}_{2}$

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