

**PO₂X···PX₃/PH₂X (X = F, Cl, Br, CH₃, NH₂)复合物中
π-hole 磷键作用的电子密度拓扑分析**

王月红 李晓艳 曾艳丽 孟令鹏 张雪英*

(河北师范大学化学与材料科学学院, 河北省无机纳米材料重点实验室, 石家庄 050024)

**Topological Analyses of Electron Density on π-hole Pnicogen Bonds
in PO₂X···PX₃/PH₂X (X = F, Cl, Br, CH₃, NH₂) Complexes**

WANG Yue-Hong LI Xiao-Yan ZENG Yan-Li MENG Ling-Peng

ZHANG Xue-Ying*

(Key Laboratory of Inorganic Nano-Materials of Hebei Province, College of Chemistry and Material Sciences,
Hebei Normal University, Shijiazhuang 050024, P. R. China)

*Corresponding author. Email: xueyingzhang@mail.hebtu.edu.cn; Tel: +86-311-80787427.

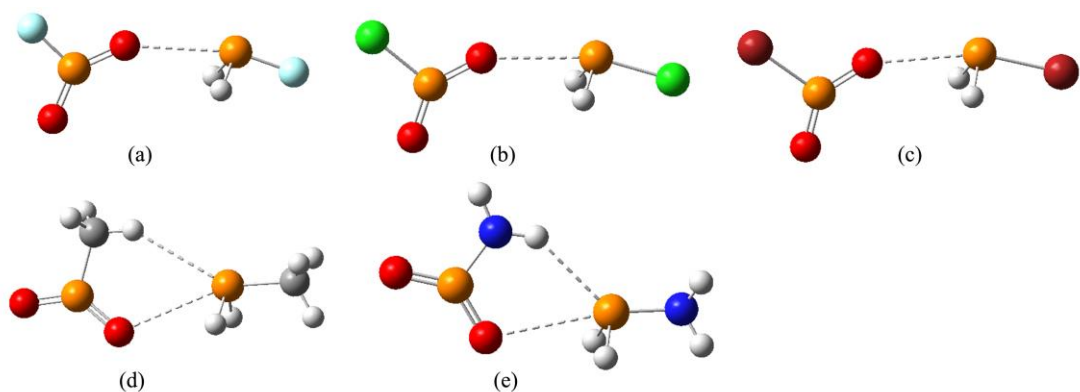


图 S1 (a)FO₂P ··· PH₂F (b)ClO₂P ··· PH₂Cl (c)BrO₂P ··· PH₂Br (d)H₃CO₂P ··· PH₂CH₃ 和 (e)H₂NO₂P ··· PH₂NH₂ 的稳定构型图

Fig.S1 Optimized geometries of the σ -hole pnictogen-bonded complexes (a)FO₂P ··· PH₂F (b)ClO₂P ··· PH₂Cl (c)BrO₂P ··· PH₂Br (d)H₃CO₂P ··· PH₂CH₃ and (e)H₂NO₂P ··· PH₂NH₂

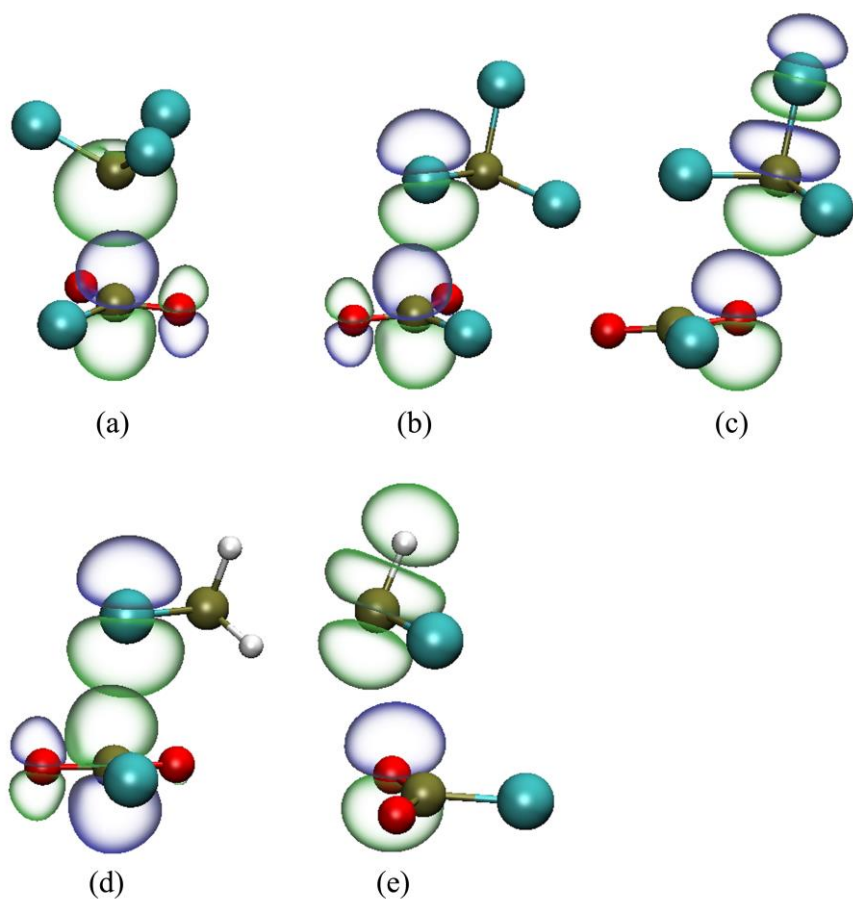


图 S2 复合物 PO₂Cl ··· PCl₃(A)(a)、PO₂Cl ··· PCl₃(B) (b)(c)和 PO₂Cl ··· PH₂Cl(B)(d)(e) 的 NBO 轨道图

Fig.S2 NBO orbital maps of PO₂Cl ··· PCl₃(A)(a)、 PO₂Cl ··· PCl₃(B)(b)(c) and PO₂Cl ··· PH₂Cl(B)(d)(e) complexes

表 S1 π -hole 磷键复合物的 Wiberg bond index 分析

Table S1 Wiberg bond index analysis of π -hole pnictogen-bonded complexes

Complexes	BCPs	WBI	Complexes	BCPs	WBI
$P_dO_2F \cdots P_sF_3(A)$	$P_d \cdots P_s$	0.0316	$P_dO_2F \cdots P_sH_2F(A)$	$P_d \cdots P_s$	0.5733
$P_dO_2Cl \cdots P_sCl_3(A)$	$P_d \cdots P_s$	0.0511	$P_dO_2Cl \cdots P_sH_2Cl(A)$	$P_d \cdots P_s$	0.4843
$P_dO_2Br \cdots P_sBr_3(A)$	$P_d \cdots P_s$	0.0610	$P_dO_2Br \cdots P_sH_2Br(A)$	$P_d \cdots P_s$	0.4600
$P_dO_2CH_3 \cdots P_s(CH_3)_3(A)$	$P_d \cdots P_s$	0.5977	$P_dO_2CH_3 \cdots P_sH_2CH_3(A)$	$P_d \cdots P_s$	0.3735
$P_dO_2NH_2 \cdots P_s(NH_2)_3(A)$	$P_d \cdots P_s$	0.6179	$P_dO_2NH_2 \cdots P_sH_2NH_2(A)$	$P_d \cdots P_s$	0.4915
	$O \cdots H$	0.0064		$O \cdots H$	0.0072
	$N \cdots H$	0.0050			
$P_dO_2F \cdots P_sF_3(B)$	$P_d \cdots F$	0.0142	$P_dO_2F \cdots P_sH_2F(B)$	$P_d \cdots F$	0.0509
$P_dO_2Cl \cdots P_sCl_3(B)$	$P_d \cdots Cl$	0.0242	$P_dO_2Cl \cdots P_sH_2Cl(B)$	$P_d \cdots Cl$	0.0425
	$O \cdots P_s$	0.0108		$O \cdots P_s$	0.0052
	$Cl \cdots Cl$	0.0006			
$P_dO_2Br \cdots P_sBr_3(B)$	$P_d \cdots Br$	0.0296	$P_dO_2Br \cdots P_sH_2Br(B)$	$P_d \cdots Br$	0.0442
	$O \cdots P_s$	0.0122		$O \cdots P_s$	0.0051
	$Br \cdots Br$	0.0008			
$P_dO_2NH_2 \cdots P_s(NH_2)_3(B)$	$P_d \cdots N$	0.3934	$P_dO_2NH_2 \cdots P_sH_2NH_2(B)$	$P_d \cdots N$	0.3372
	$O \cdots H$	0.0151			