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$H_2XP\cdots SHY$ 复合物中磷键与硫键的理论研究

刘玉震　　黎安勇*

(西南大学化学化工学院, 重庆　400715)

Theoretical Analysis of Pnicogen and Chalcogen Bonds in $H_2XP\cdots SHY$ Complexes

LIU Yu-Zhen　　LI An-Yong*

(*School of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, P. R. China*)

*Corresponding author. Email: aylifnsy@swu.edu.cn; Tel: +86-23-68252360

表 S1　各单体和复合物的相关结构参数

Table S1　Some structural parameters of all monomers and complexes

Pnicogen bond	*L*(PH)/nm	*L*(PX)/nm	*υ*(PX)/cm^{-1}	*L*(P⋯S)/nm	∠XPS/(°)
H_2FP	0.1416(0.1430)	0.1622(0.1673)	809(778.9)		
H_2ClP	0.1413(0.1427)	0.2076(0.2114)	523.2(501.2)		
H_2BrP	0.1413(0.1427)	0.2234(0.2272)	415.5(396.9)		
H_2FP-SH_2(P1)	0.1415(0.1429)	0.1631(0.1683)	780.2(753.2)	0.3192	166.4
H_2ClP-SH_2(P1)	0.1412(0.1425)	0.2090(0.2129)	500.5(480.2)	0.3283	165.9
H_2BrP-SH_2(P1)	0.1411(0.1425)	0.2249(0.2288)	(380.2)	0.3280	166.2
H_2FP-SHF(P2, P3)	0.1415(0.1429)	0.1629(0.1679)	(760.4)	0.3096	170.0
H_2ClP-SHF(P2)	0.1412(0.1426)	0.2086(0.2123)	(487.9)	0.3233	167.8
H_2BrP-SHF(P2)	0.1412(0.1425)	0.2244(0.2282)	(387.2)	0.3236	168.5
H_2ClP-SHCl(P3)	0.1412(0.1425)	0.2087(0.2125)	(485.2)	0.3232	166.9
H_2BrP-SHBr(P3)	0.1412(0.1425)	0.2246(0.2285)	(383.6)	0.3220	167.9
Chalcogen bond	*L*(SH)/nm	*L*(SY)/nm	*υ*(SY)/cm^{-1}	*L*(P⋯S)/nm	∠YSP/(°)
HFS	0.1339(0.1353)	0.1634(0.1678)	797.8(781.8)		
HClS	0.1338(0.1352)	0.2039(0.2077)	550.4(524.7)		
HBrS	0.1339(0.1353)	0.2188(0.2227)	441.9(417.5)		
HFS-PH_3(S1)	0.1336(0.1350)	0.1670(0.1705)	684.8(701.6)	0.2737	173.9
HClS-PH_3(S1)	0.1336(0.1350)	0.2062(0.2097)	507.1(487.7)	0.3079	173.1
HBrS-PH_3(S1)	0.1336(0.1350)	0.2208(0.2246)	(389.6)	0.3121	173.2
HFS-PH_2F(S2, S3)	0.1335(0.1351)	0.170(0.1702)	(705.3)	0.2463	176.7
HClS-PH_2F(S2)	0.1337(0.1351)	0.2061(0.2091)	(497.0)	0.3026	176.7
HBrS-PH_2F(S2)	0.1337(0.1351)	0.2207(0.2241)	(396.9)	0.3074	177.0
HClS-PH_2Cl(S3)	0.1337(0.1351)	0.2059(0.2092)	(493.8)	0.3026	177.3
HBrS-PH_2Br(S3)	0.1338(0.1352)	0.2205(0.2242)	(392.9)	0.3064	177.8

L: bond length: *υ*: frequency. The results in brackets are calculated at MP2/aug-cc-pVDZ level, the other data are calculated at MP2/aug-cc-pVTZ level.