

Supporting Information to the paper

Lone pair– π interactions: a new supramolecular bond?

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Table S1 Lp– π close contacts found in the CSD between different unusual atoms **LP** and uncommon six-membered heteroaromatic rings

Ring	Number of lp– π contacts found				Mean atom LP –centroid distance (<i>D</i> , Å)				Relative standard deviation of the data set (RSD, %)			
	R–Cl	R=O	R–Sb(R')–R''	R–Bi(R')–R''	R–Cl	R=O	R–Sb(R')–R''	R–Bi(R')–R''	R–Cl	R=O	R–Sb(R')–R''	R–Bi(R')–R''
Benzene (R1)			42	22			3.268	3.173			4	6
Phosphinine	1				3.455				n.a. ^a			
Arsinine		1				3.237				n.a.		
1,3,5-Trithiine		1				3.033				n.a.		
2,4-S,6-P-1,3,5-triazine	1	2			3.469	3.318			n.a.	n.a.		
2,4,6-S-1,3,5-triazine	1				3.303				n.a.			
2-P-1,3,5-triazine	2				3.324				n.a.			

^a The relative standard deviation (RSD) of the data set can not be calculated if the number of contacts found is ≤ 2 . n.a. stands for “not available”