

Supplementary data for the article:

Milovanović, M. M.; Andrić, J. M.; Medaković, V. B.; Djukic, J.-P.; Zarić, S. D. Investigation of Interactions in Lewis Pairs between Phosphines and Boranes by Analyzing Crystal Structures from the Cambridge Structural Database. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials* **2018**, *74* (3), 255–263. <https://doi.org/10.1107/S2052520618003736>



STRUCTURAL SCIENCE  
CRYSTAL ENGINEERING  
MATERIALS

**Volume 74 (2018)**

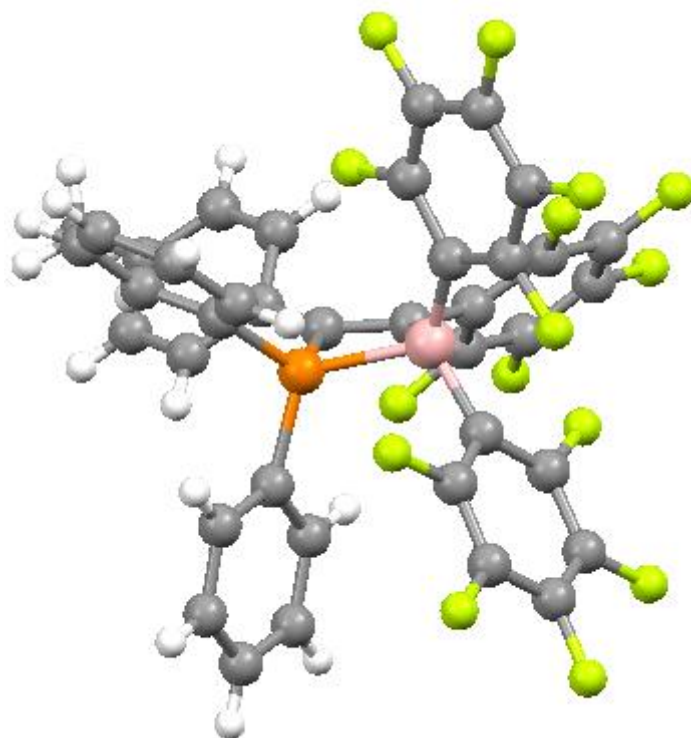
**Supporting information for article:**

**INVESTIGATION OF INTERACTIONS IN LEWIS PAIRS BETWEEN  
PHOSPHINES AND BORANES BY ANALYZING CRYSTAL  
STRUCTURES FROM CAMBRIDGE STRUCTURAL DATABASE**

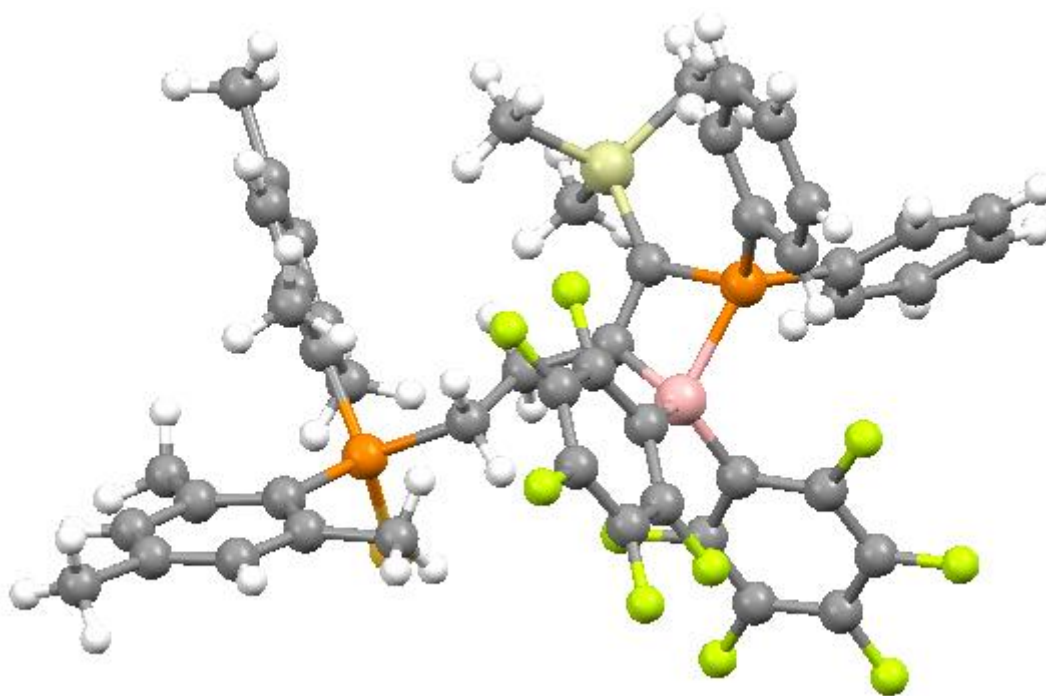
**Milan M. Milovanović, Jelena M. Andrić, Vesna B. Medaković, Jean-Pierre  
Djukic and Snežana D. Zarić**

### S1. The crystal structures of experimental and evaluated FLPs

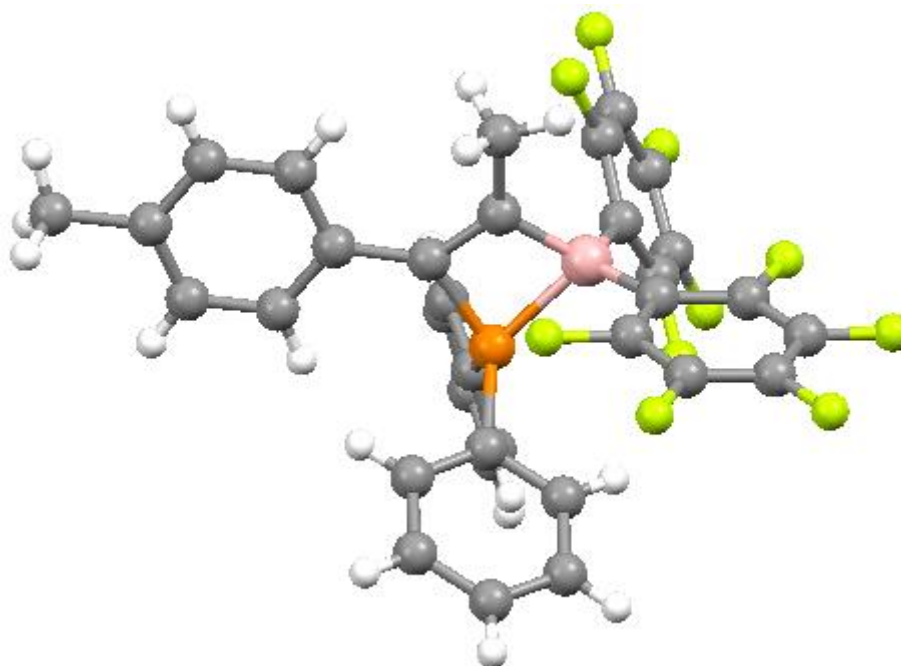
The representation of crystal structures of both, **experimental** (Figures S2 – S11) and **evaluated** FLPs (Figures S12 – S21) are given to illustrate considered structures.



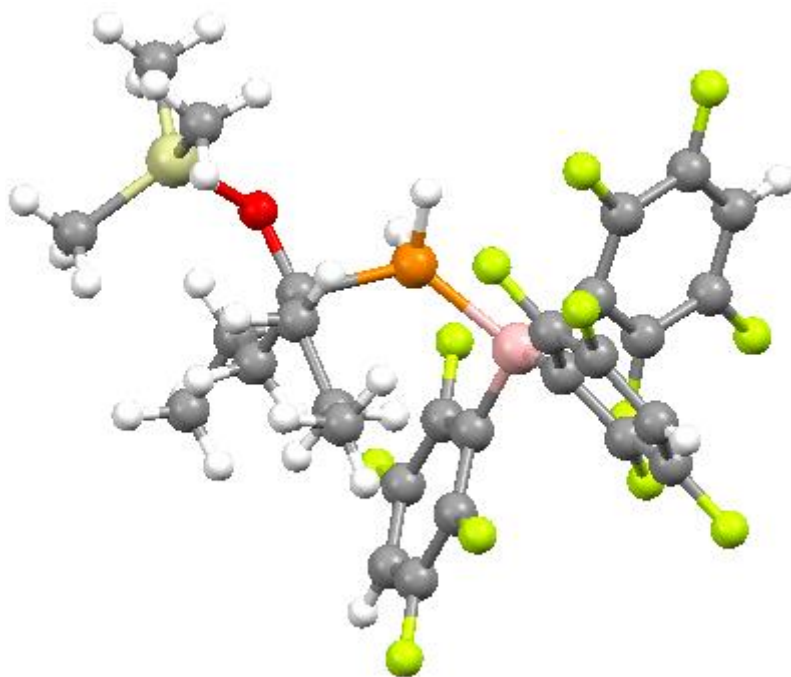
**Figure S1** Crystal structure **SEZKAL** (Ekkert *et al.*, 2013). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **experimental** FLP.



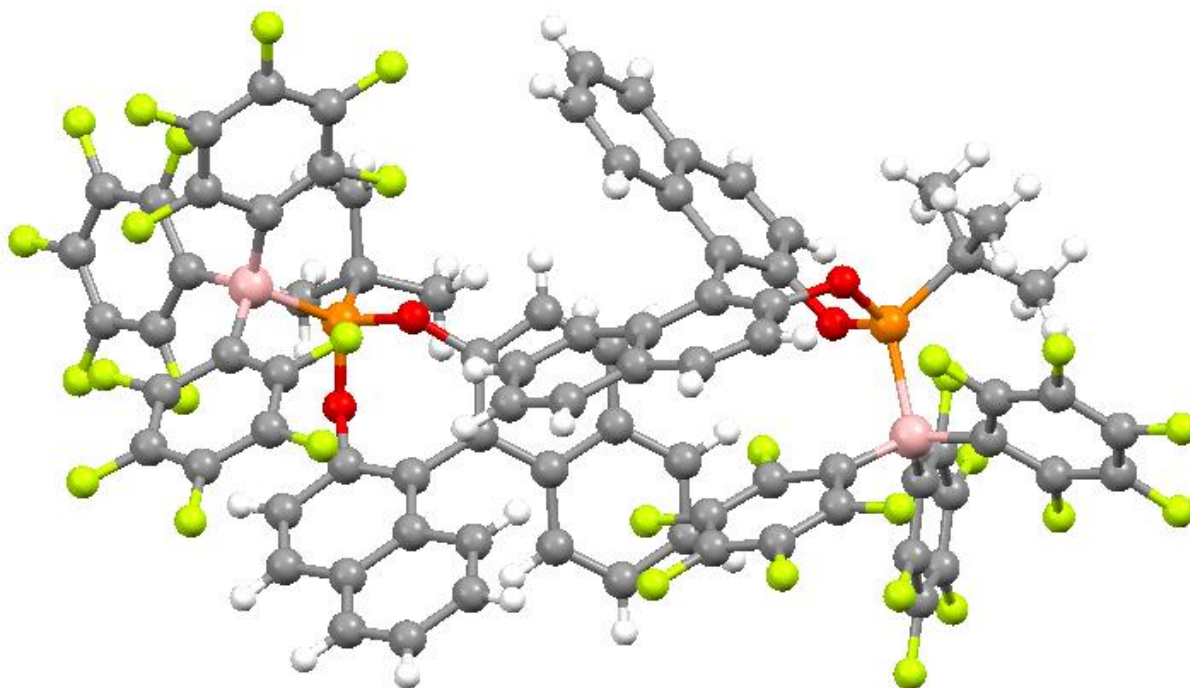
**Figure S2** Crystal structure **FUWKUF** (Liedtke *et al.*, 2014). P: orange; B: pink; F: yellow; Si: light green; Cl: green; C: gray; H: white. This structure corresponds to the **experimental** FLP.



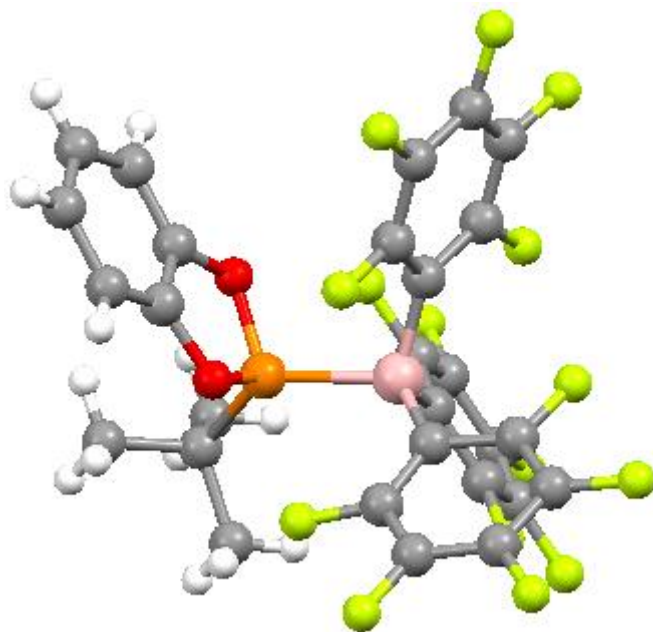
**Figure S3** Crystal structure **SEZJUE** (Ekkert *et al.*, 2013). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **experimental** FLP.



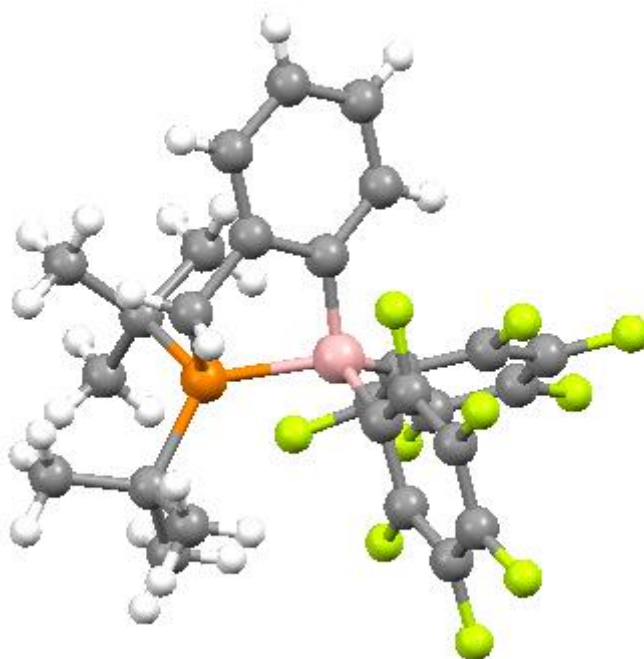
**Figure S4** Crystal structure **ODUJUU** (Takeuchi *et al.*, 2013). P: orange; B: pink; F: yellow; Si: light green; O: red; C: gray; H: white. This structure corresponds to the **experimental** FLP.



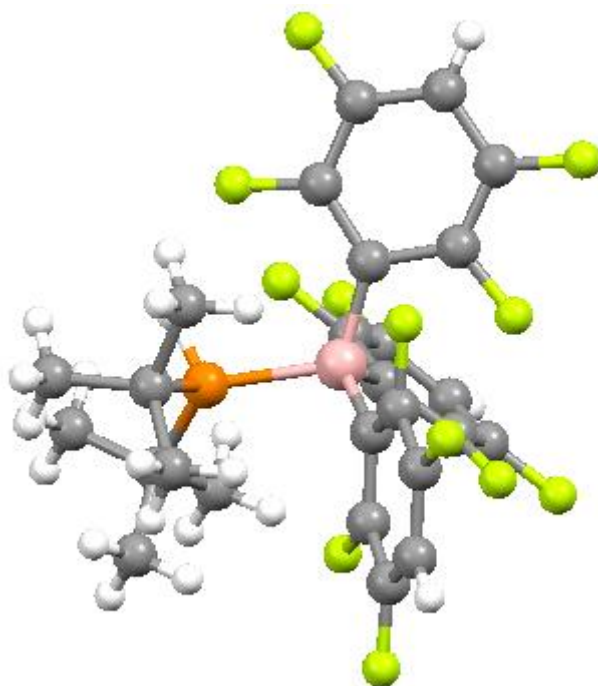
**Figure S5** Crystal structure **FAPGIO** (Caputo *et al.*, 2013) P: orange; B: pink; F: yellow; O: red; C: gray; H: white. This structure corresponds to the **experimental** FLP.



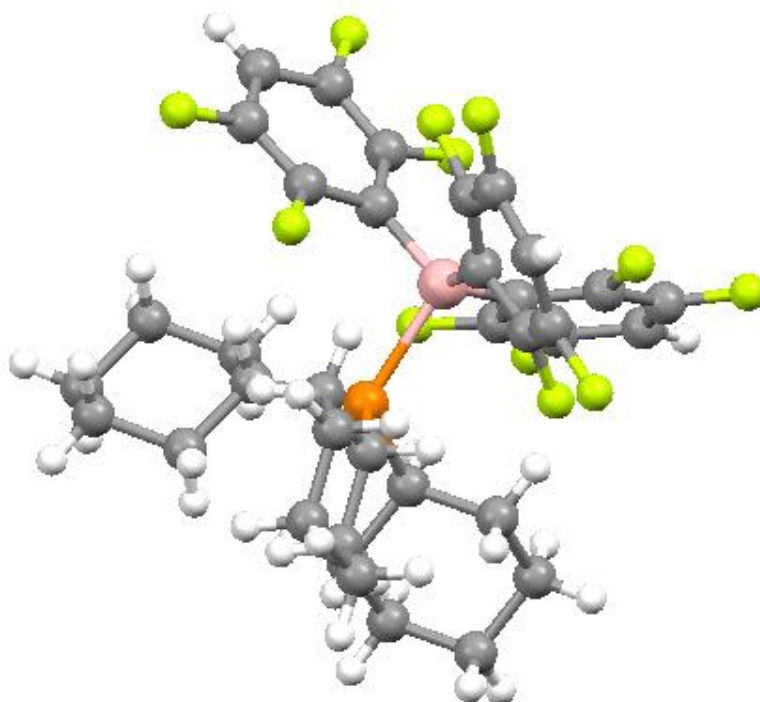
**Figure S6** Crystal structure **FAPGEK** (Caputo *et al.*, 2013). P: orange; B: pink; F: yellow; O: red; C: gray; H: white. This structure corresponds to the **experimental** FLP.



**Figure S7** Crystal structure **OSUZEI** (Heiden *et al.*, 2011). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **experimental** FLP.

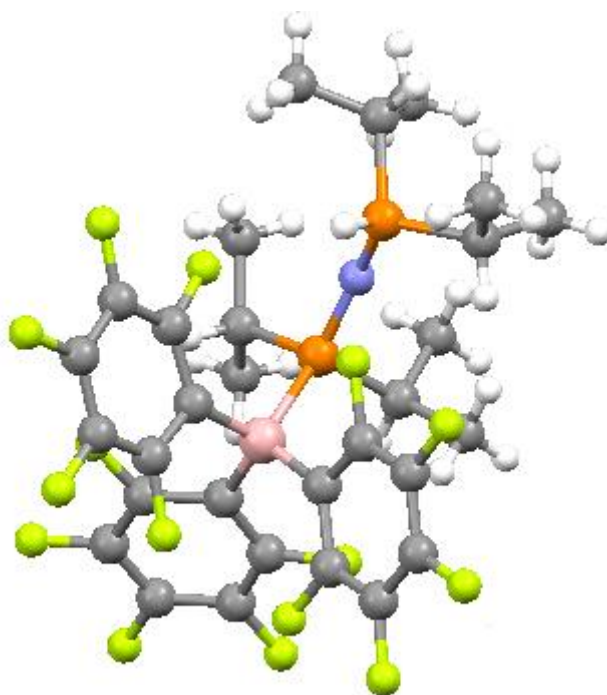


**Figure S8** Crystal structure **OLAJOB** (Ullrich *et al.*, 2010). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **experimental FLP**.

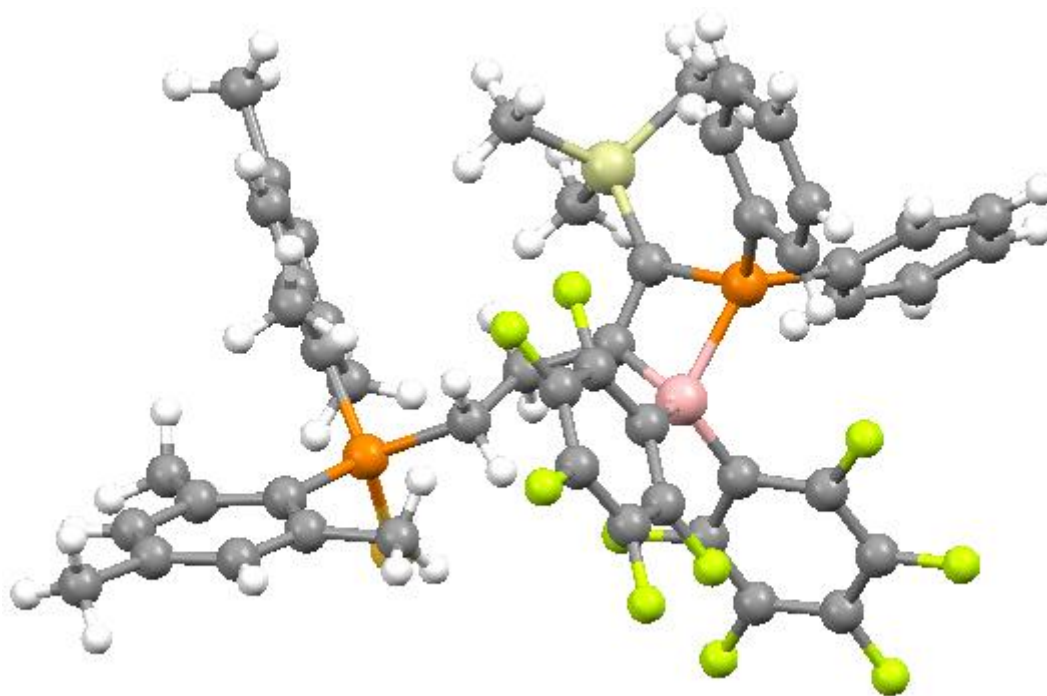


**Figure S9** Crystal structure **OLAJUH** (Ullrich *et al.*, 2010). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **experimental FLP**.



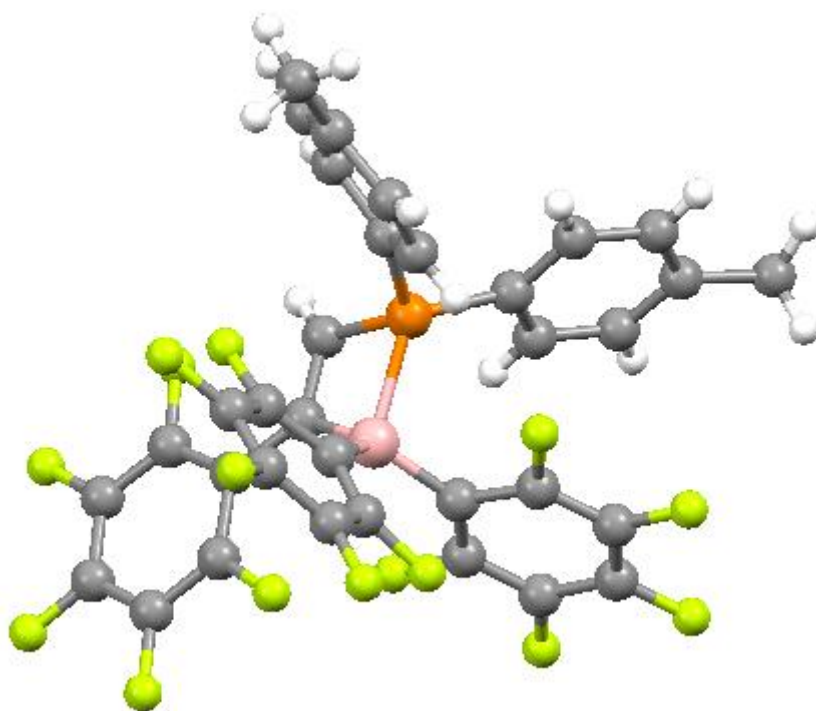


**Figure S10** Crystal structure **MIKDER** (Barry *et al.*, 2013). P: orange; B: pink; F: yellow; the nitrogen atoms - blue, C: gray; H: white. This structure corresponds to the **experimental** FLP.

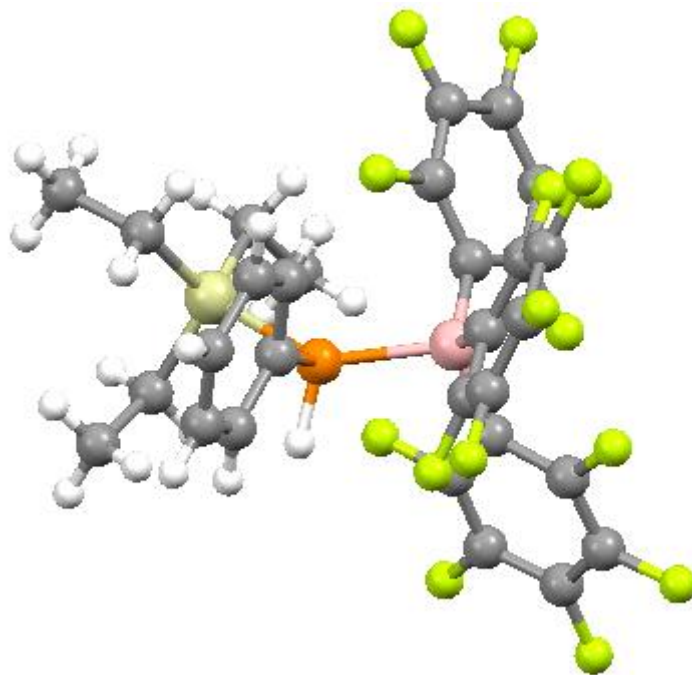


**Figure S11** Crystal structure **FUWLEQ** (Liedtke *et al.*, 2014). P: orange; B: pink; F: yellow; Si: light green; the sulfur brown, C: gray; H: white. This structure corresponds to the **evaluated** FLP.

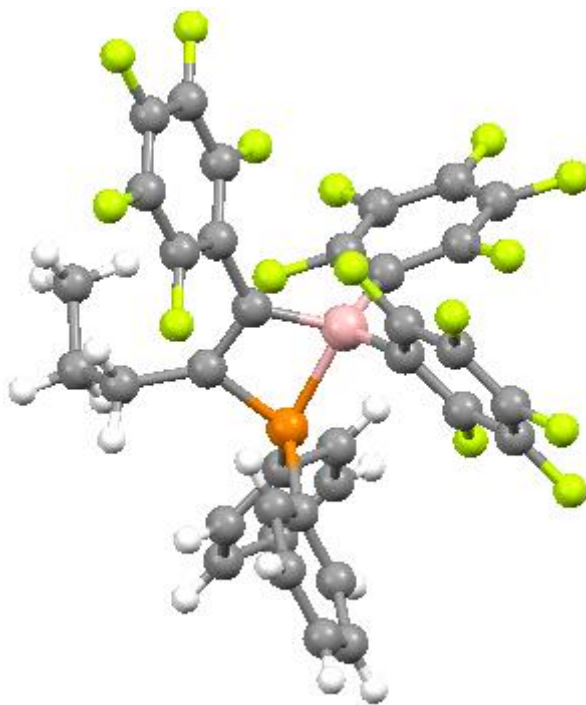




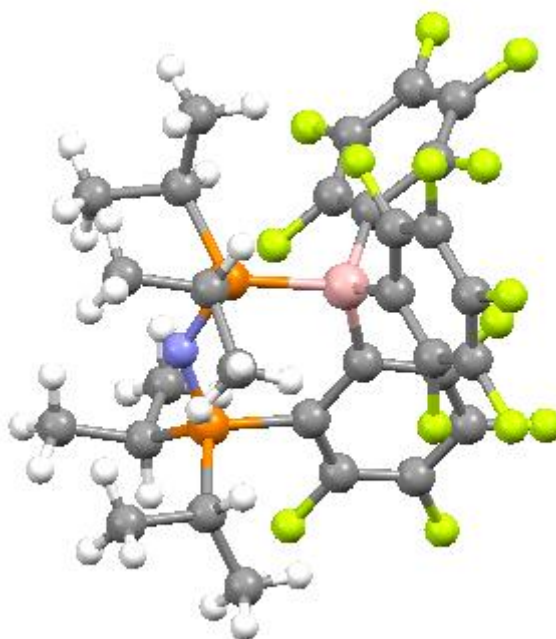
**Figure S12** Crystal structure **BIRXAD** (Yu *et al.*, 2013). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **evaluated** FLP.



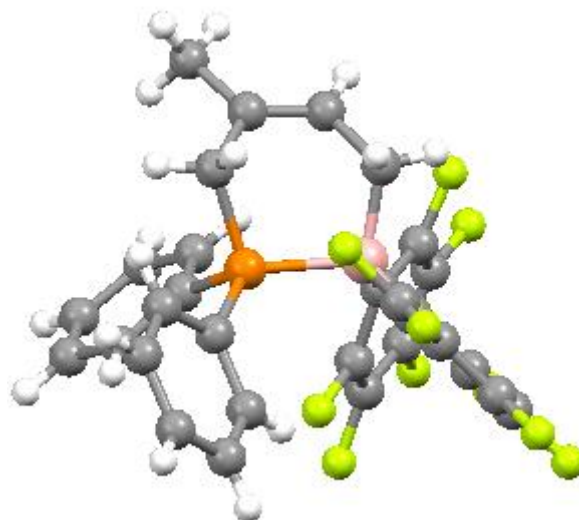
**Figure S13** Crystal structure **XUPZAK** (Geier & Stephan, 2010). P: orange; B: pink; F: yellow; Si: light green; C: gray; H: white. This structure corresponds to the **evaluated** FLP.



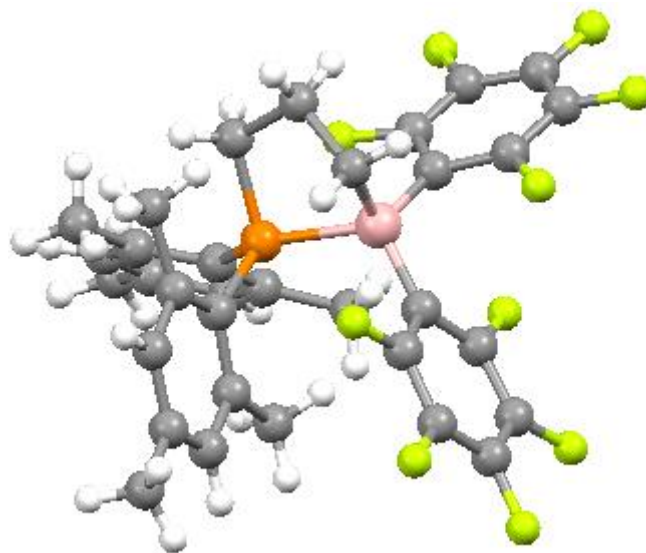
**Figure S14** Crystal structure **EWETAC** (Ekkert *et al.*, 2011). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **evaluated** FLP.



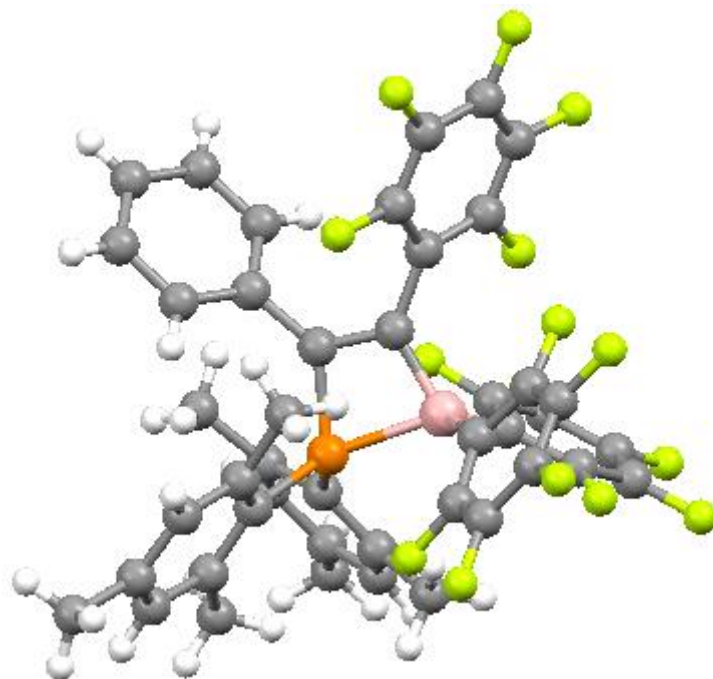
**Figure S15** Crystal structure **MIKCUG** (Barry *et al.*, 2013). P: orange; B: pink; F: yellow; N: blue; C: gray; H: white. This structure corresponds to the **evaluated** FLP.



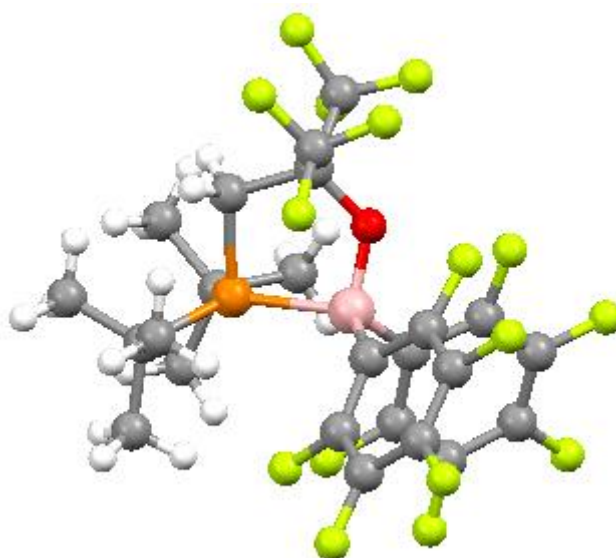
**Figure S16** Crystal structure **ROVLAR** (Moquist *et al.*, 2015). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **evaluated** FLP.



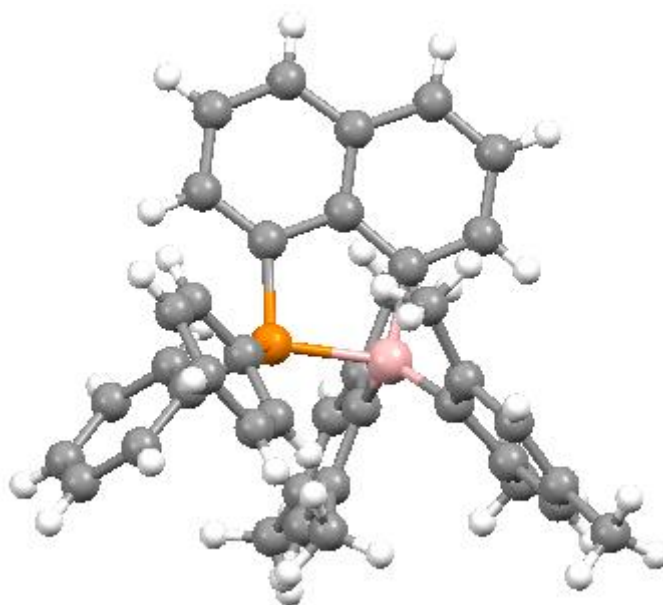
**Figure S17** Crystal structure **YORPAX** (Spies *et al.*, 2009). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **evaluated** FLP.



**Figure S18** Crystal structure **EWESUV** (Ekkert *et al.*, 2011). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **evaluated** FLP.



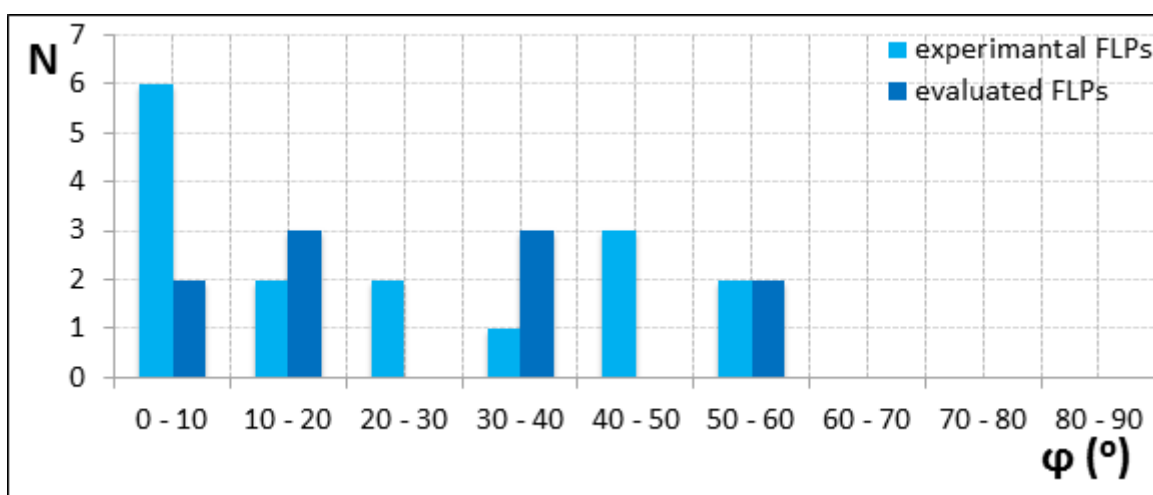
**Figure S19** Crystal structure **TACHAI** (Chapman *et al.*, 2010). P: orange; B: pink; F: yellow; O: red; C: gray; H: white. This structure corresponds to the **evaluated** FLP.



**Figure S20** Crystal structure **SIGVUB01** (Beckmann *et al.*, 2013). P: orange; B: pink; C: gray; H: white. This structure corresponds to the **evaluated** FLP.

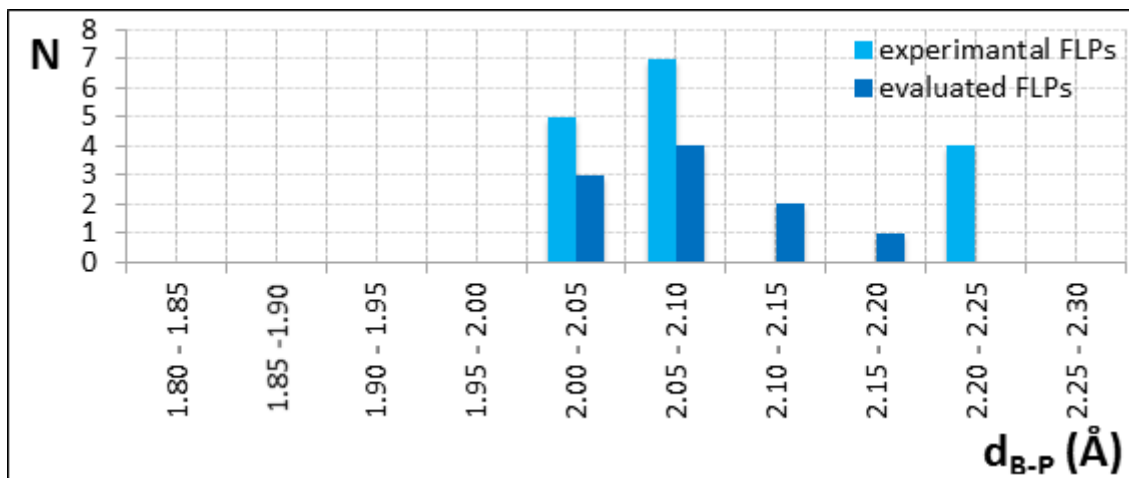
## S2. Analysis of the data from CSD for FLPs

The separated distributions of the studied geometrical parameters ( $\varphi$ ,  $d_{B-P}$ ,  $r$ ,  $R$  (Figure 1)) of both, **experimental** and **evaluated** FLPs are given to show similarity in the distribution and to confirm the reliability of the way of choosing the **evaluated** FLPs.

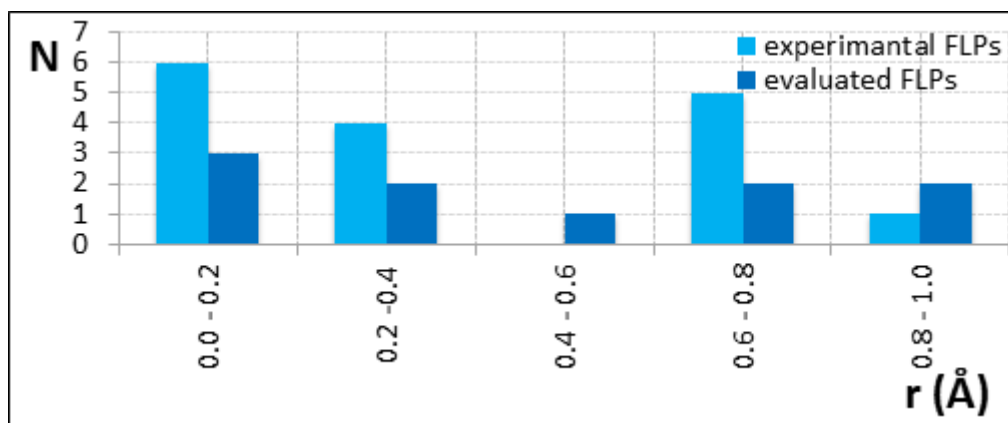


**Figure S21** The distribution of the dihedral angle  $\varphi$  (Figure 1) of the interacting molecules in the contacts in the FLPs set. The notation **experimental FLPs** represents the structures for which *there is* experimental evidence in the literature that they belong to the class of frustrated Lewis pairs. The notation **evaluated FLPs** represents the structures for which *there is no* experimental evidence in the

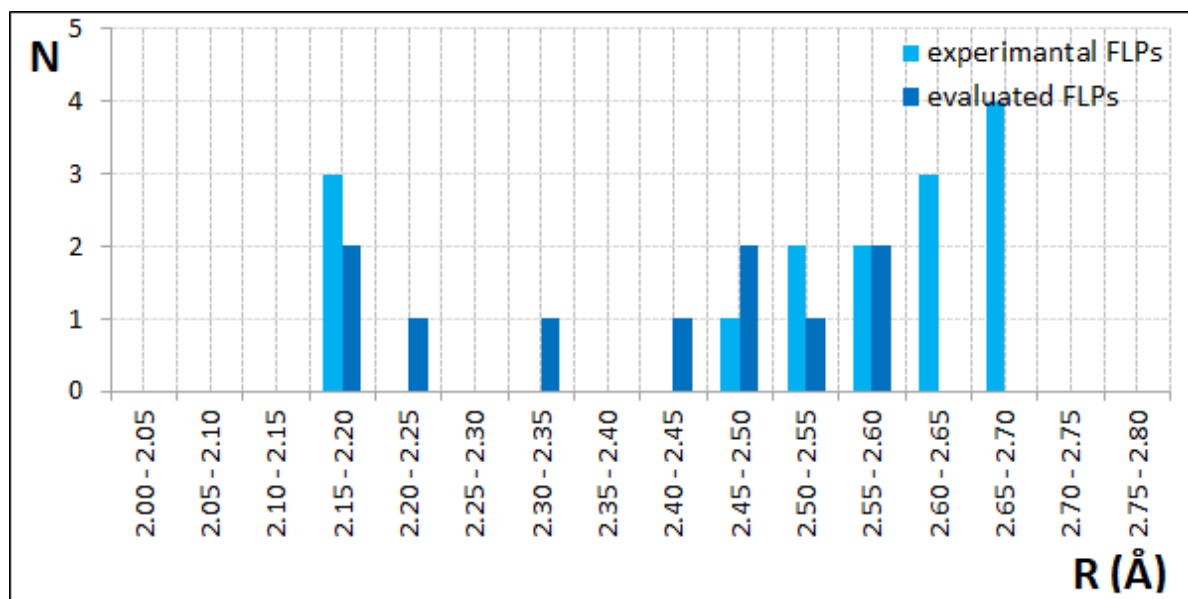
literature that they belong to the class of frustrated Lewis pairs, but they are structurally very similar to the documented ones.



**Figure S22** The distribution of the distance between phosphorus and boron atoms  $d_{B-P}$  (Figure 1) of the interacting molecules in the FLPs set. The notation **experimental FLPs** represents the structures for which *there is* experimental evidence in the literature that they belong to the class of frustrated Lewis pairs. The notation **evaluated FLPs** represents the structures for which *there is no* experimental evidence in the literature that they belong to the class of frustrated Lewis pairs, but they are structurally very similar to the documented ones.



**Figure S23** The distribution of the offset distance  $r$  (Figure 1) of the interacting molecules in the FLPs set. The notation **experimental FLPs** represents the structures for which *there is* experimental evidence in the literature that they belong to the class of frustrated Lewis pairs. The notation **evaluated FLPs** represents the structures for which *there is no* experimental evidence in the literature that they belong to the class of frustrated Lewis pairs, but they are structurally very similar to the documented ones.



**Figure S24** The distribution of the normal distance  $R$  (Figure 1) of the interacting molecules in the FLPs set. The notation **experimental FLPs** represents the structures for which *there is* experimental evidence in the literature that they belong to the class of frustrated Lewis pairs. The notation **evaluated FLPs** represents the structures for which *there is no* experimental evidence in the literature that they belong to the class of frustrated Lewis pairs, but they are structurally very similar to the documented ones.