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Supporting information for article:

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

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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.

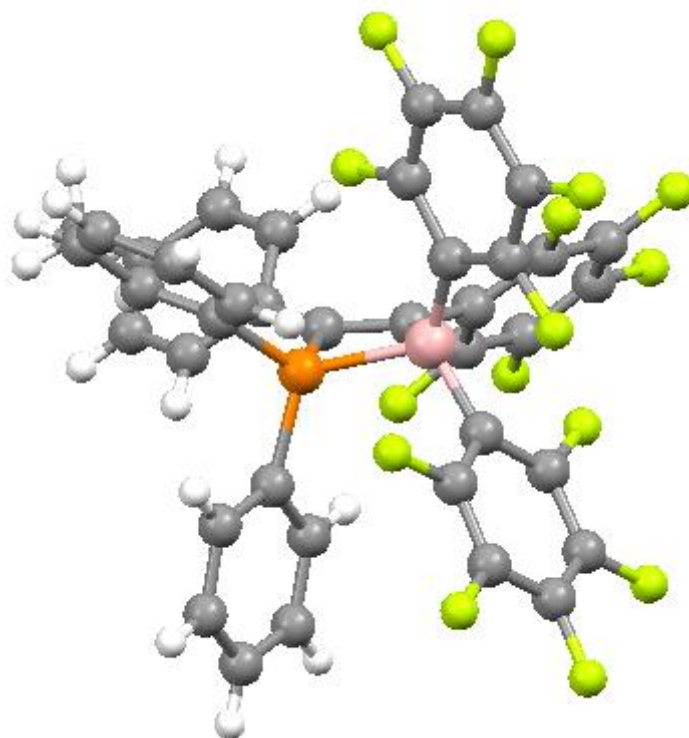


Figure S1 Crystal structure **SEZKAL** (Ekkert *et al.*, 2013). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **experimental** FLP.

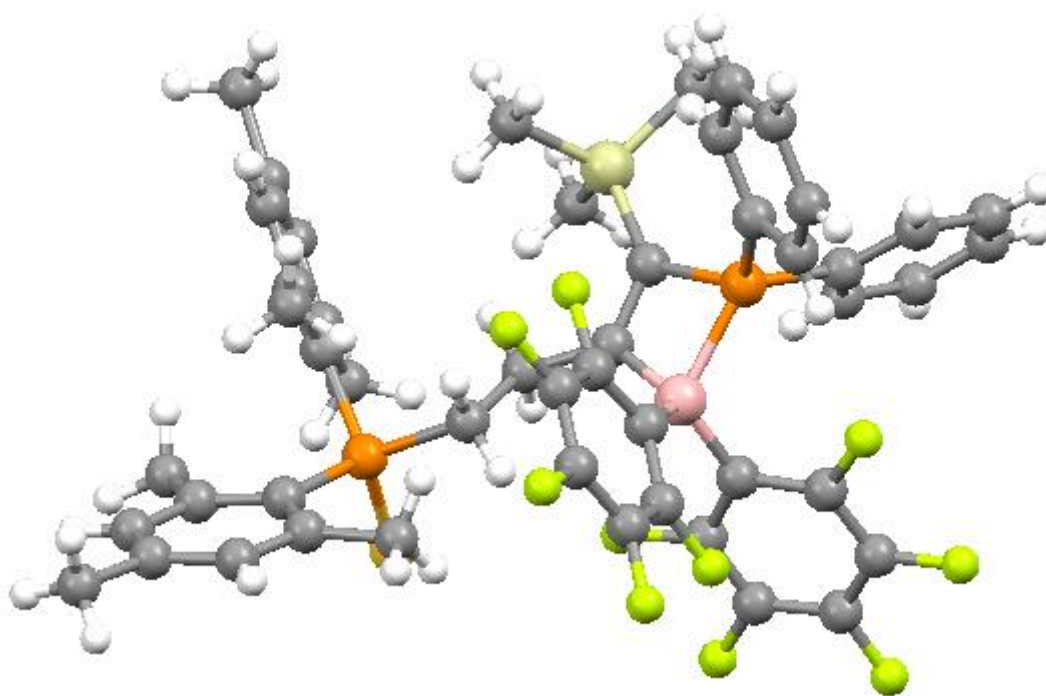


Figure S2 Crystal structure **FUWKUF** (Liedtke *et al.*, 2014). P: orange; B: pink; F: yellow; Si: light green; Cl: green; C: gray; H: white. This structure corresponds to the **experimental** FLP.

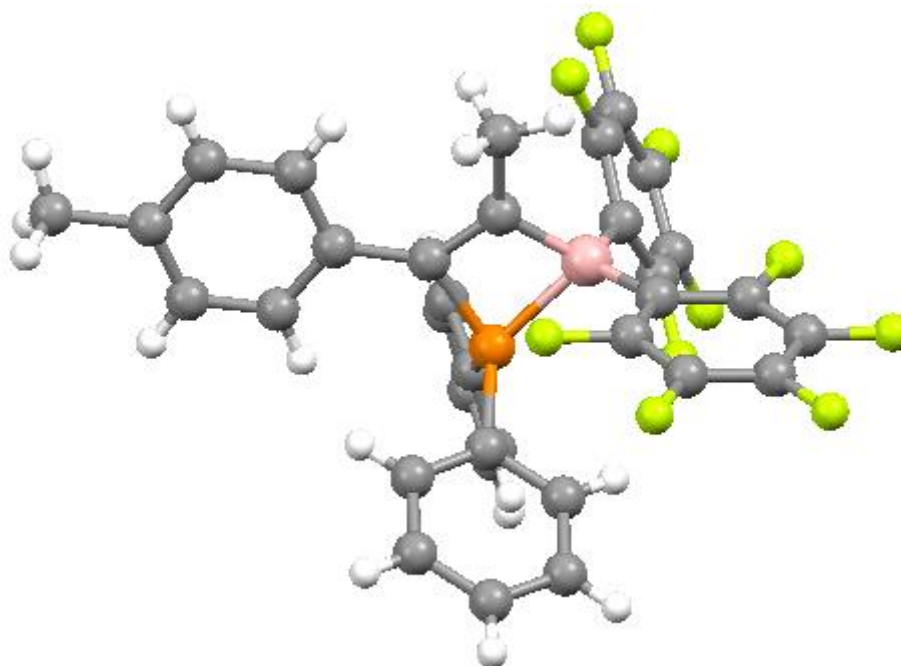


Figure S3 Crystal structure **SEZJUE** (Ekkert *et al.*, 2013). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **experimental** FLP.

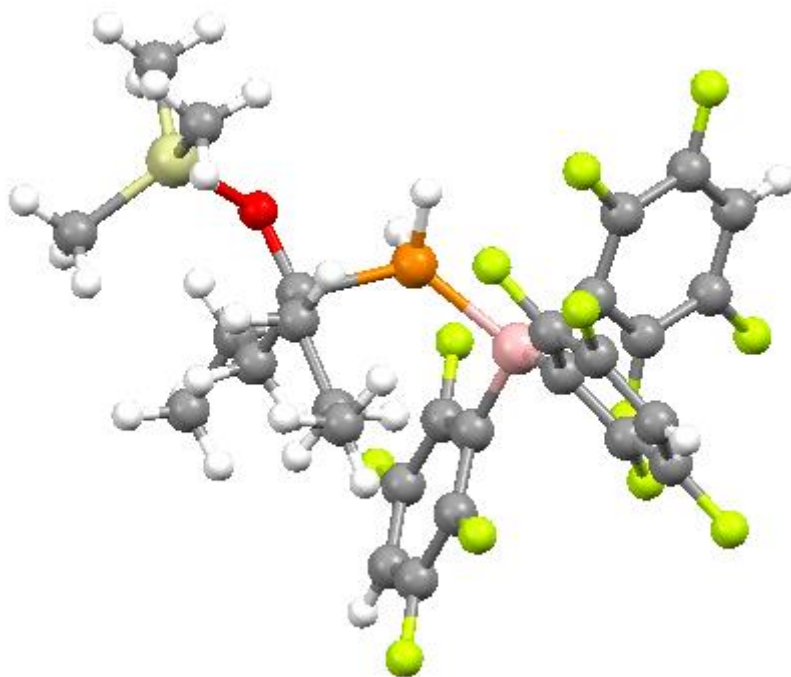


Figure S4 Crystal structure **ODUJUU** (Takeuchi *et al.*, 2013). P: orange; B: pink; F: yellow; Si: light green; O: red; C: gray; H: white. This structure corresponds to the **experimental FLP**.

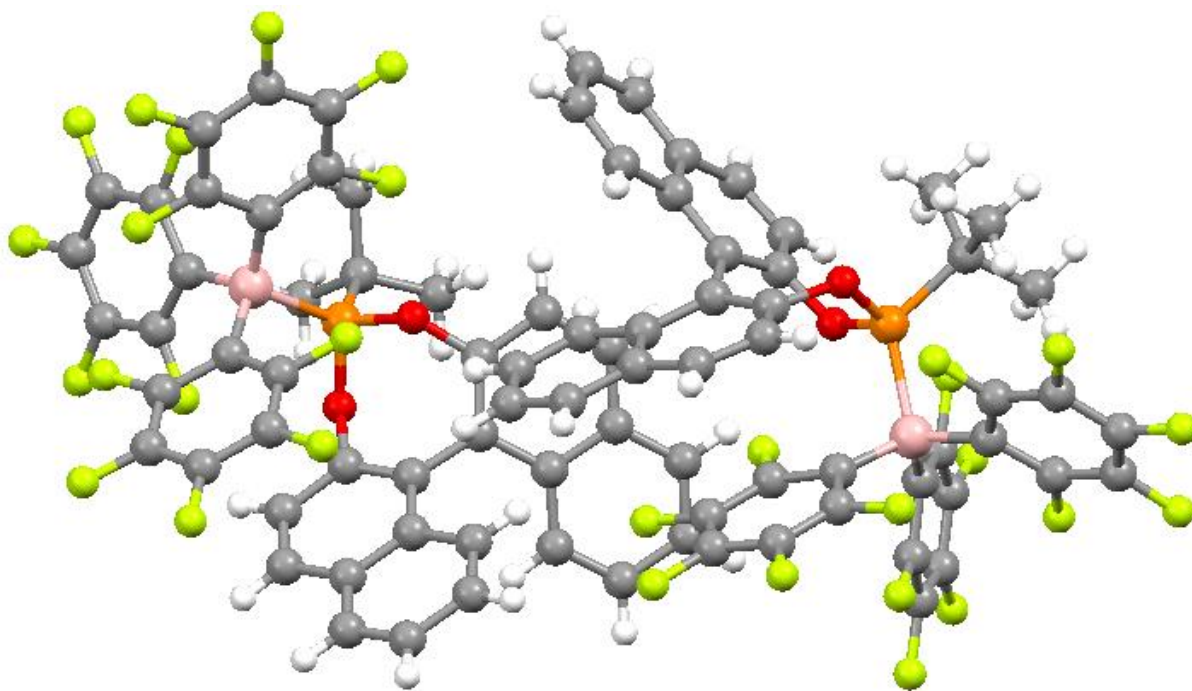


Figure S5 Crystal structure **FAPGIO** (Caputo *et al.*, 2013) P: orange; B: pink; F: yellow; O: red; C: gray; H: white. This structure corresponds to the **experimental FLP**.

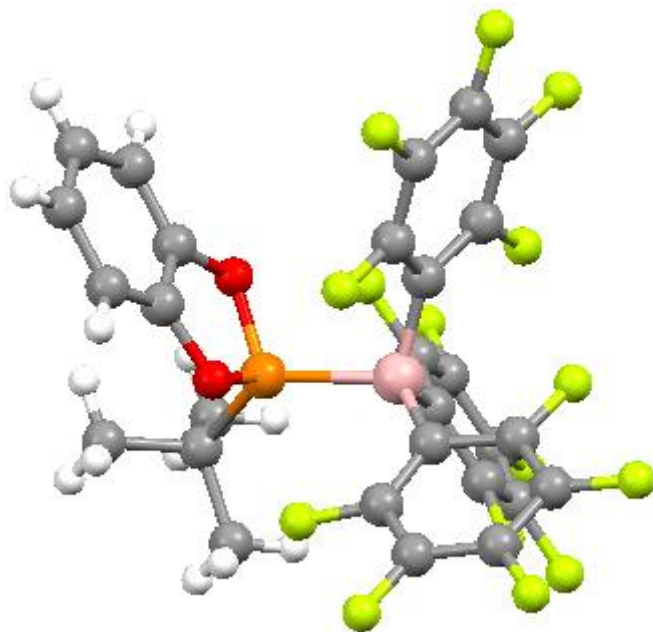


Figure S6 Crystal structure **FAPGEK** (Caputo *et al.*, 2013). P: orange; B: pink; F: yellow; O: red; C: gray; H: white. This structure corresponds to the **experimental FLP**.

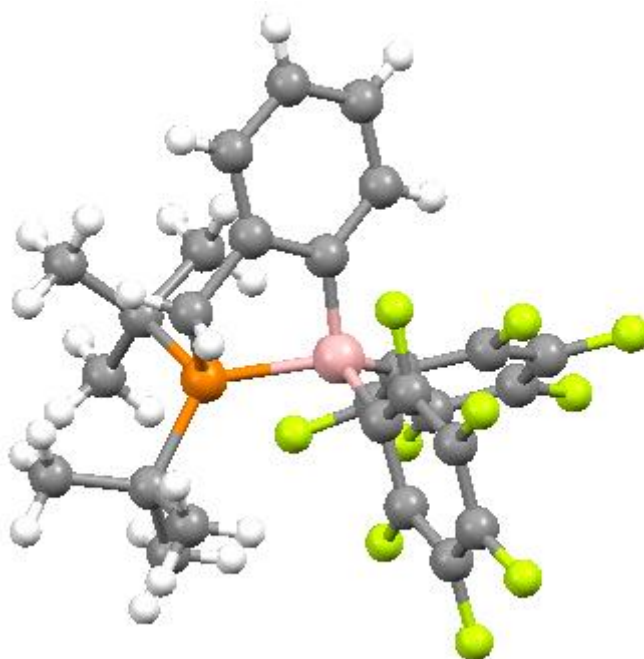


Figure S7 Crystal structure **OSUZEI** (Heiden *et al.*, 2011). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **experimental FLP**.

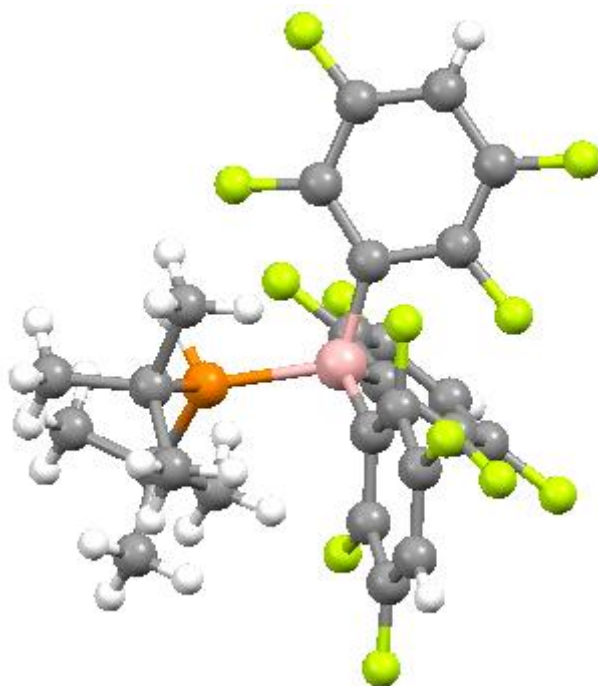


Figure S8 Crystal structure **OLAJOB** (Ullrich *et al.*, 2010). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **experimental FLP**.

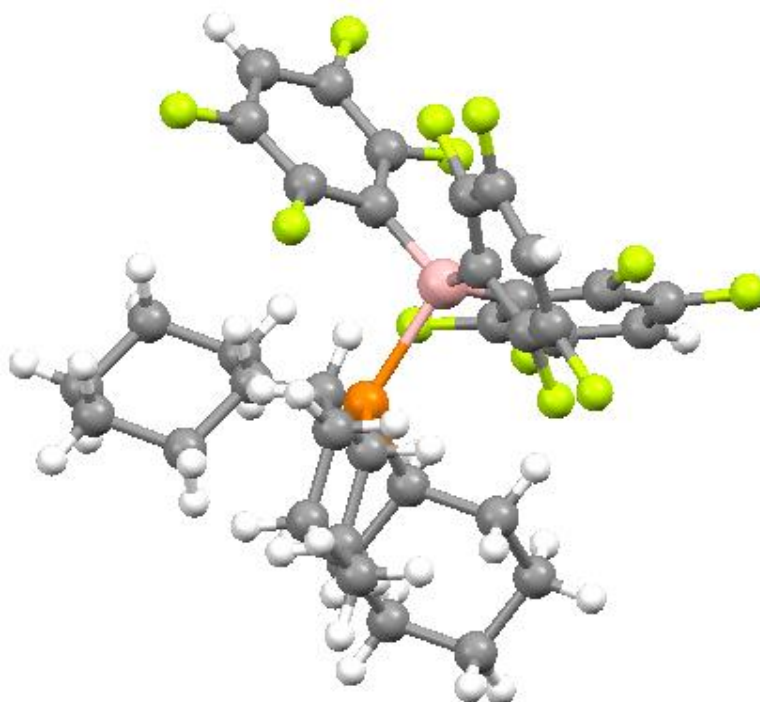


Figure S9 Crystal structure **OLAJUH** (Ullrich *et al.*, 2010). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **experimental FLP**.

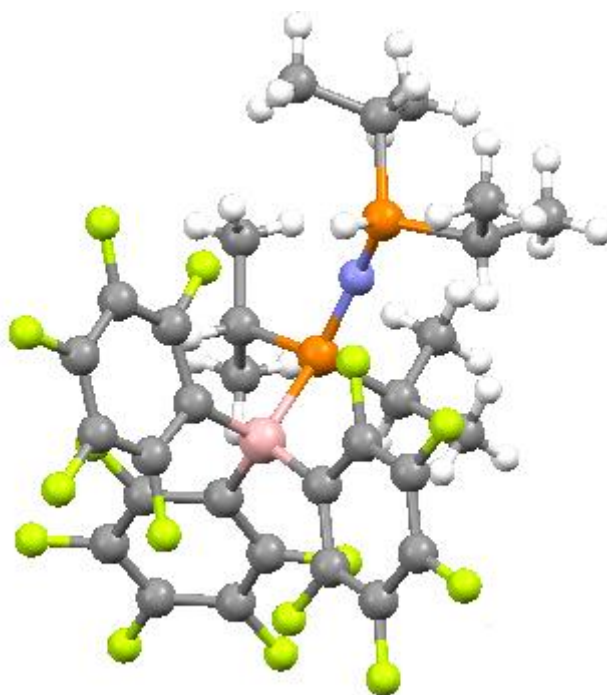


Figure S10 Crystal structure **MIKDER** (Barry *et al.*, 2013). P: orange; B: pink; F: yellow; the nitrogen atoms - blue, C: gray; H: white. This structure corresponds to the **experimental** FLP.

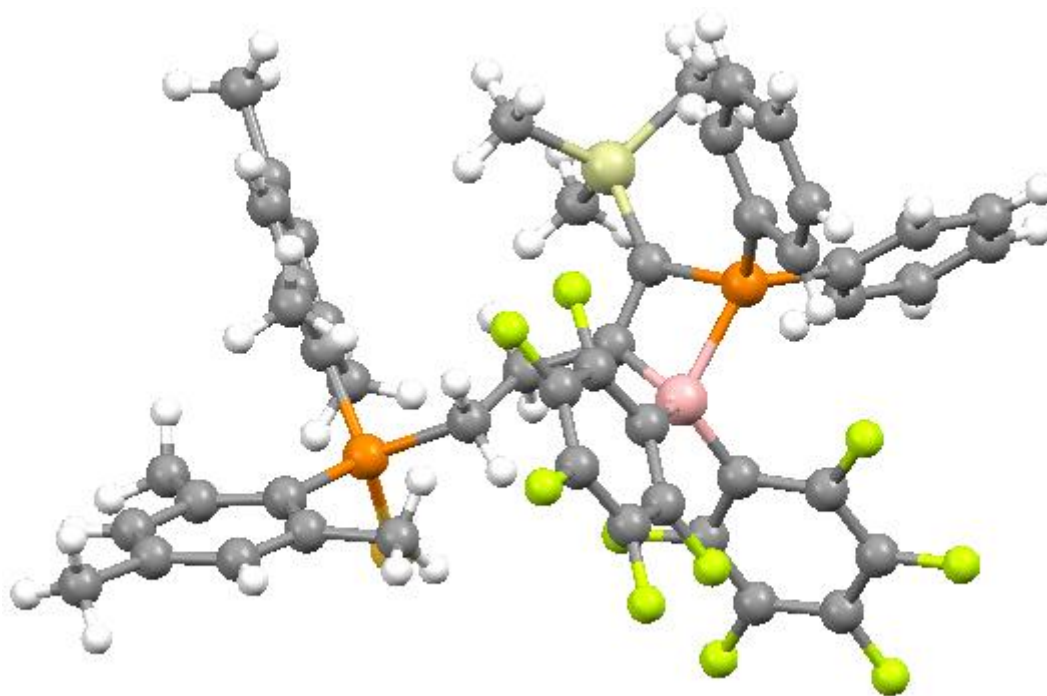


Figure S11 Crystal structure **FUWLEQ** (Liedtke *et al.*, 2014). P: orange; B: pink; F: yellow; Si: light green; the sulfur brown, C: gray; H: white. This structure corresponds to the **evaluated** FLP.

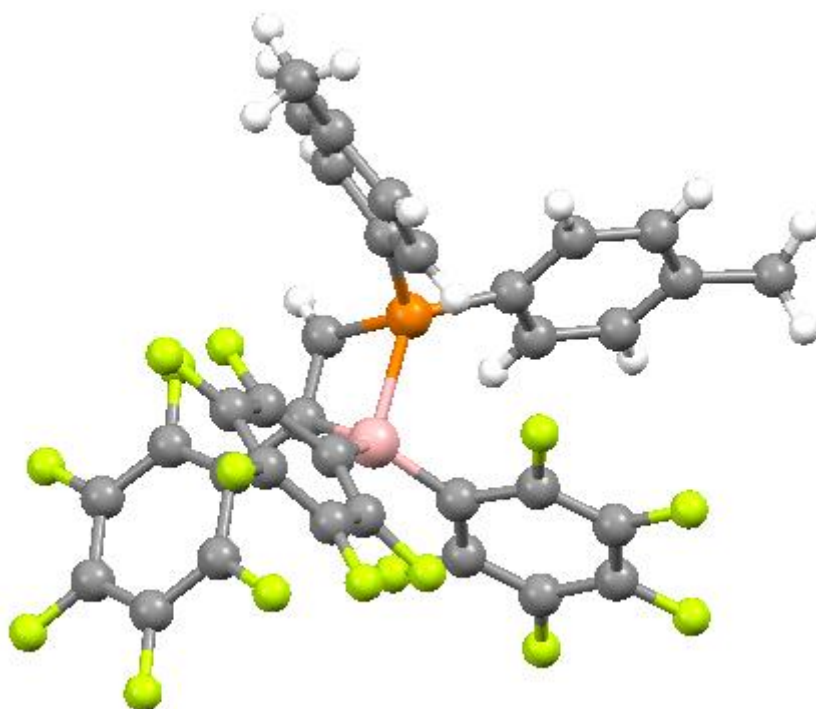


Figure S12 Crystal structure **BIRXAD** (Yu *et al.*, 2013). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **evaluated** FLP.

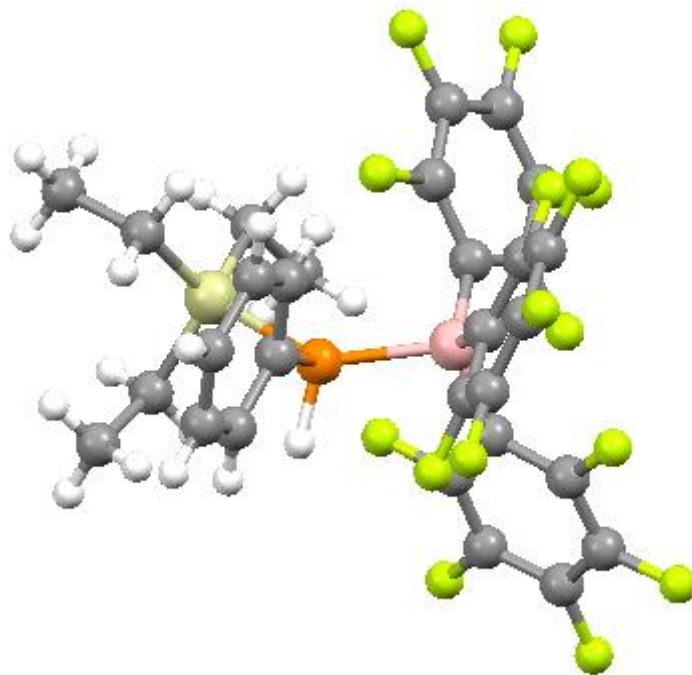


Figure S13 Crystal structure **XUPZAK** (Geier & Stephan, 2010). P: orange; B: pink; F: yellow; Si: light green; C: gray; H: white. This structure corresponds to the **evaluated** FLP.

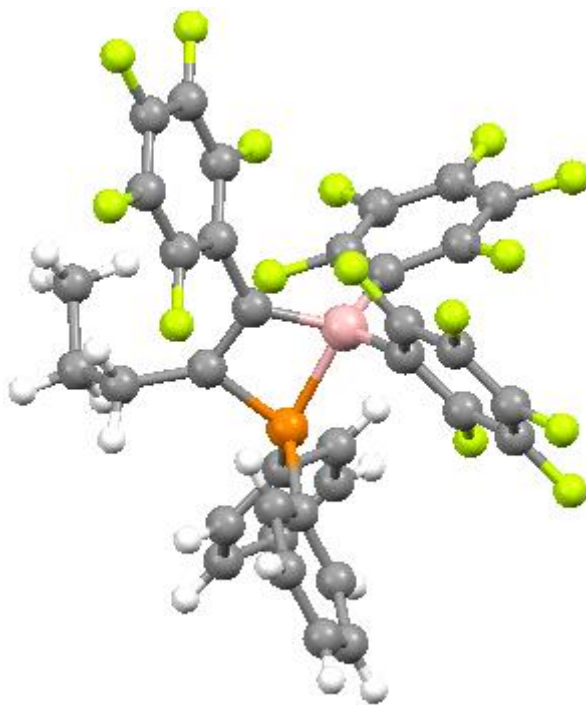


Figure S14 Crystal structure **EWETAC** (Ekkert *et al.*, 2011). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **evaluated** FLP.

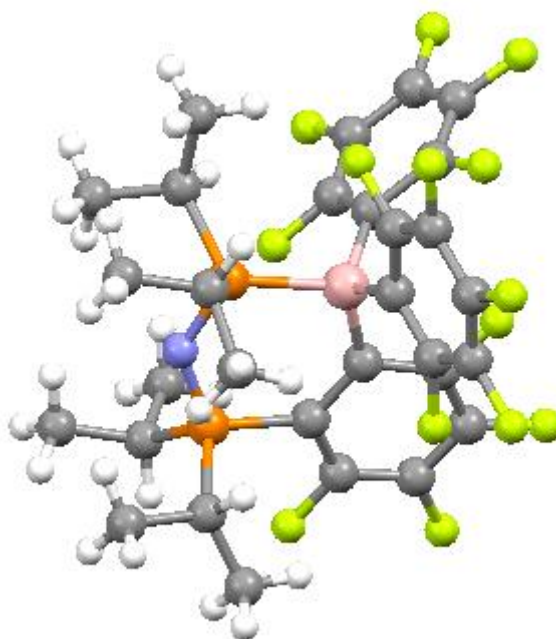


Figure S15 Crystal structure **MIKCUG** (Barry *et al.*, 2013). P: orange; B: pink; F: yellow; N: blue; C: gray; H: white. This structure corresponds to the **evaluated** FLP.

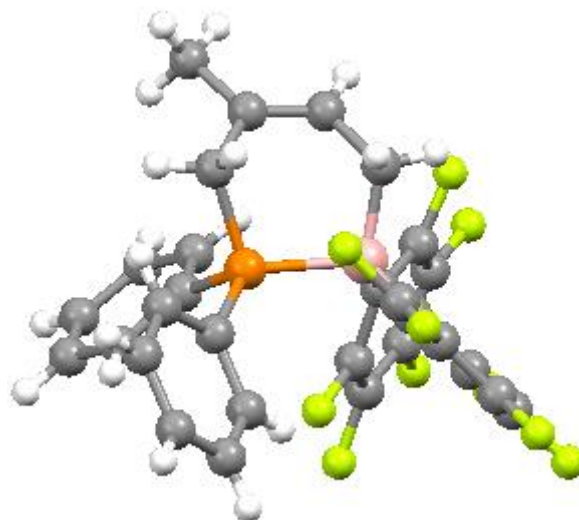


Figure S16 Crystal structure **ROVLAR** (Moquist *et al.*, 2015). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **evaluated** FLP.

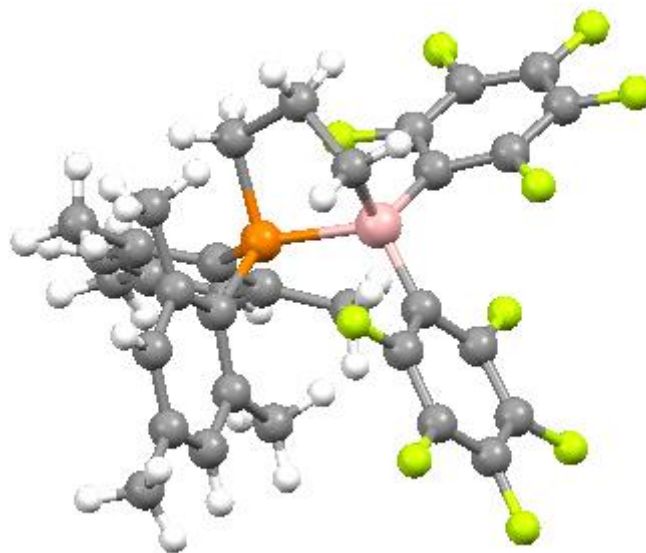


Figure S17 Crystal structure **YORPAX** (Spies *et al.*, 2009). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **evaluated** FLP.

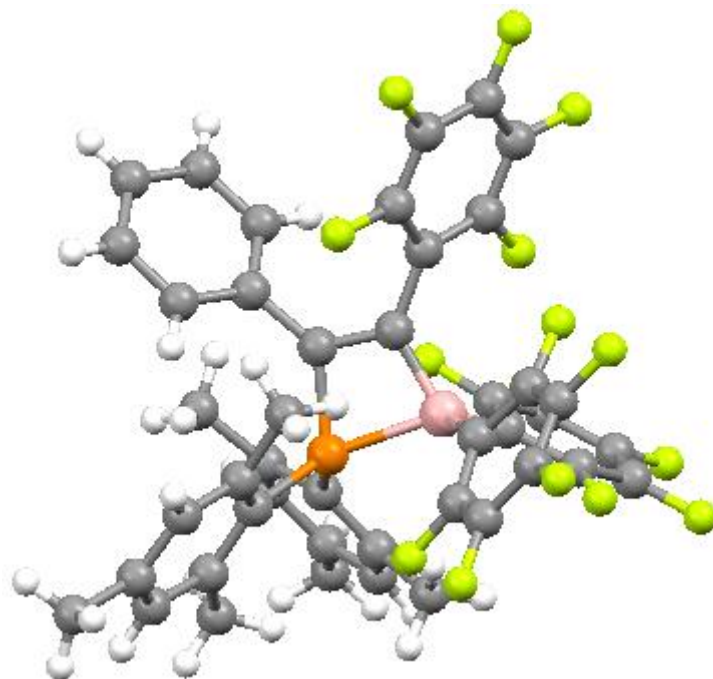


Figure S18 Crystal structure **EWESUV** (Ekkert *et al.*, 2011). P: orange; B: pink; F: yellow; C: gray; H: white. This structure corresponds to the **evaluated** FLP.

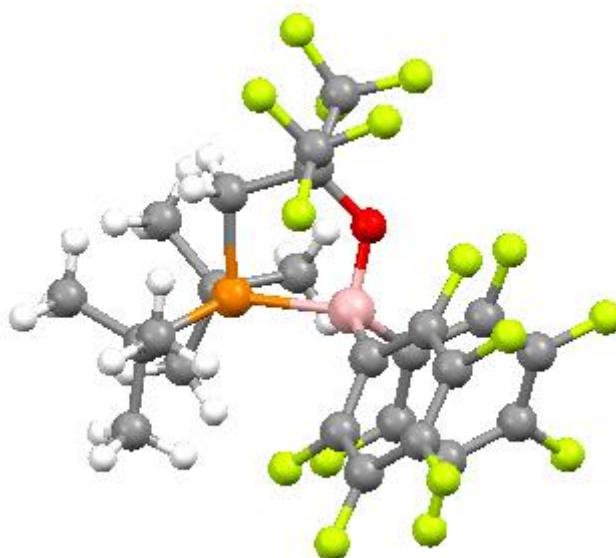


Figure S19 Crystal structure **TACHAI** (Chapman *et al.*, 2010). P: orange; B: pink; F: yellow; O: red; C: gray; H: white. This structure corresponds to the **evaluated** FLP.

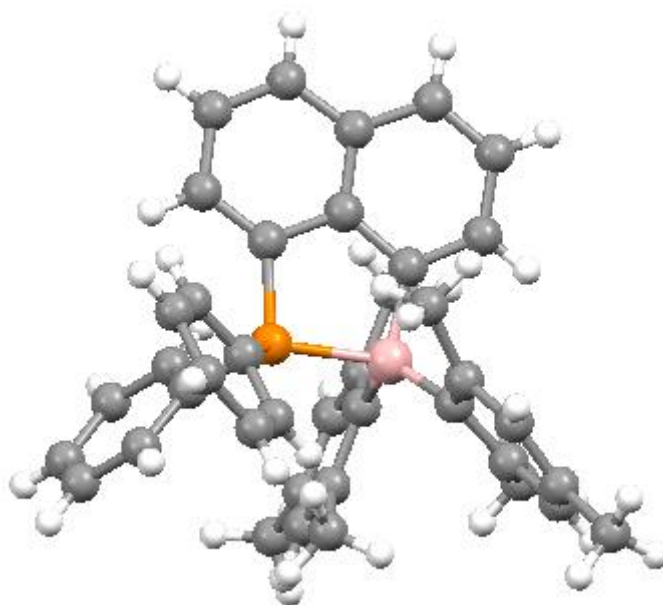


Figure S20 Crystal structure **SIGVUB01** (Beckmann *et al.*, 2013). P: orange; B: pink; C: gray; H: white. This structure corresponds to the **evaluated** FLP.

S2. Analysis of the data from CSD for FLPs

The separated distributions of the studied geometrical parameters (φ , 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.

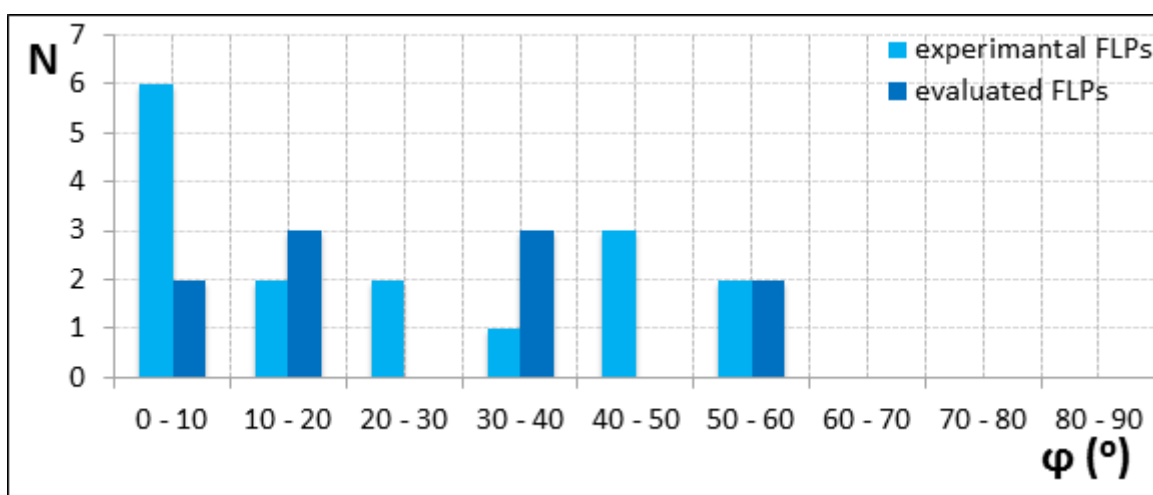


Figure S21 The distribution of the dihedral angle φ (Figure 1) of the interacting molecules in the contacts in the FLPs set. The notation **experimental FLPs** represents the structures for which *there is* experimental evidence in the literature that they belong to the class of frustrated Lewis pairs. 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.

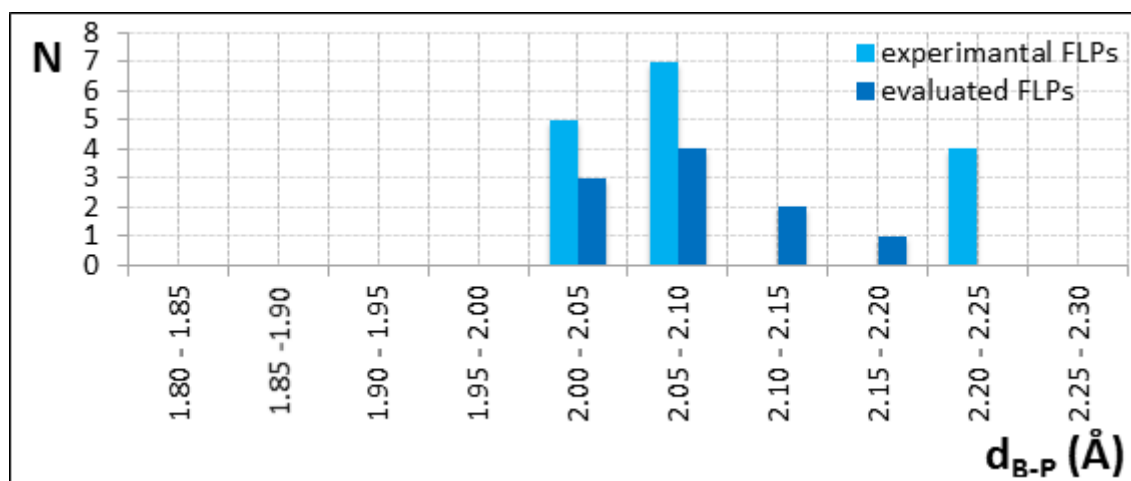


Figure S22 The distribution of the distance between phosphorus and boron atoms d_{B-P} (Figure 1) of the interacting molecules in the FLPs set. The notation **experimental FLPs** represents the structures for which *there is* experimental evidence in the literature that they belong to the class of frustrated 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.

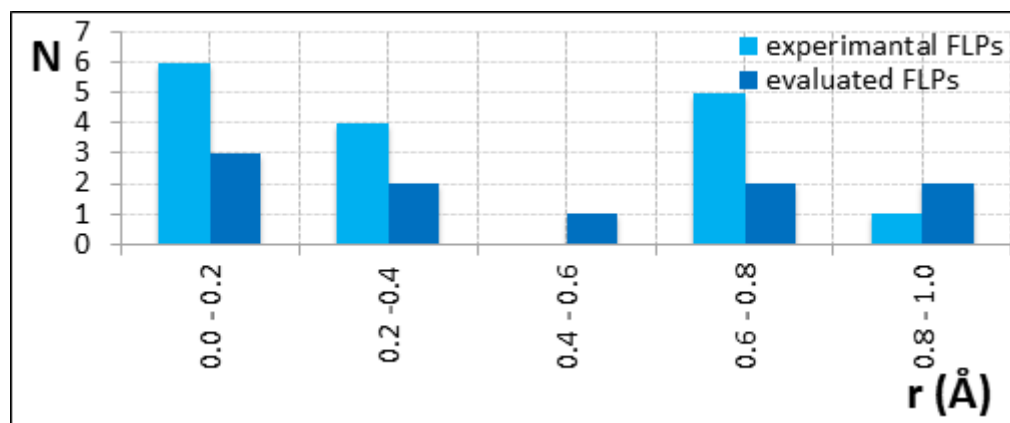


Figure S23 The distribution of the offset distance r (Figure 1) of the interacting molecules in the FLPs set. The notation **experimental FLPs** represents the structures for which *there is* experimental evidence in the literature that they belong to the class of frustrated Lewis pairs. The notation **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.

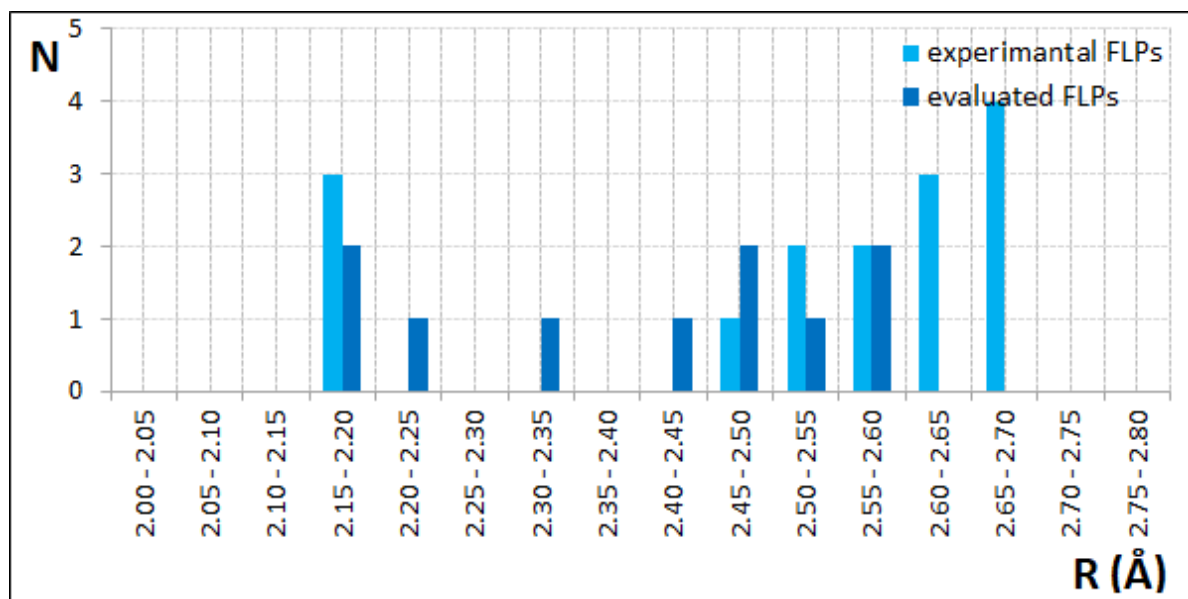


Figure S24 The distribution of the normal distance **R** (Figure 1) of the interacting molecules in the FLPs set. The notation **experimental FLPs** represents the structures for which *there is* experimental evidence in the literature that they belong to the class of frustrated Lewis pairs. The notation **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.