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π -HOLE DONOR ABILITY OF FLUORINATED IODOARENES

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Noncovalent interactions play an important role in many advanced areas of modern science spanning from supramolecular chemistry to molecular biology. While amount of studies on hydrogen bonding (HB), halogen bonding (XB), π - π -stacking, and metallophilic interactions is gradually stabilized, many novel types of noncovalent forces including, e.g., anion- π or, more generally, lone pair- π (lp- π) interactions classified in Figure 1 were recognized only recently thus providing a new tool for crystal engineering.

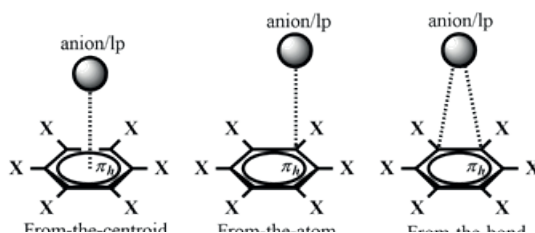


Figure 1. (Anion/lp)- π binding motifs.

In this work, we demonstrated that fluorinated electron deficient iodoarenes (FIBs) such as iodopentafluorobenzene, 1,4-diiodotetrafluorobenzene, and 1,3,5-triiodotrifluorobenzene co-crystallize with square planar platinum(II) and nickel(II) complexes, viz. $[n\text{-Bu}_4\text{N}]_2[\text{Pt}_2(\mu\text{-I}_2)\text{I}_4]$ and $[\text{Ni}\{\text{NH}=\text{C}(\text{NRR}')\text{NN}(\text{O})\}_2]$ ($\text{RR}' = \text{Me}_2$, $\text{RR}' = \text{MePh}$, $\text{RR}' = (\text{CH}_2)_5$), giving supramolecular structures held by several types of weak contacts.^{1,2} Upon analysis of noncovalent forces in the structures of obtained adducts, in addition to rather conventional HBs and XBs, we recognized hitherto unknown (anion/lp)- π interactions involving FIBs acting as π -hole donors. The types of (anion/lp)- π interactions revealed by us represent novel noncovalent bonding patterns involving FIBs and open up an avenue to the focused application of these synthons in supramolecular chemistry as building blocks exhibiting π -hole or mixed σ -hole/ π -hole donor properties.

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