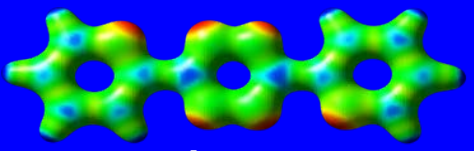
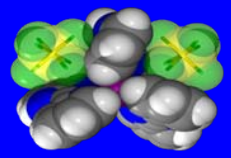
Systematic and Theoretical Studies of Anion-π Interactions for the Development of Supermolecules and New Materials

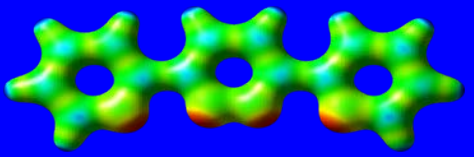
Kim R. Dunbar, Department of Chemistry, Texas A&M University



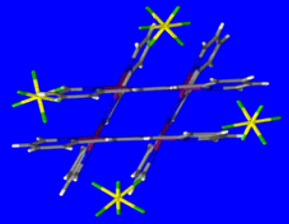
bptz



$Ag_2(bptz)_3[SbF_6]_2$

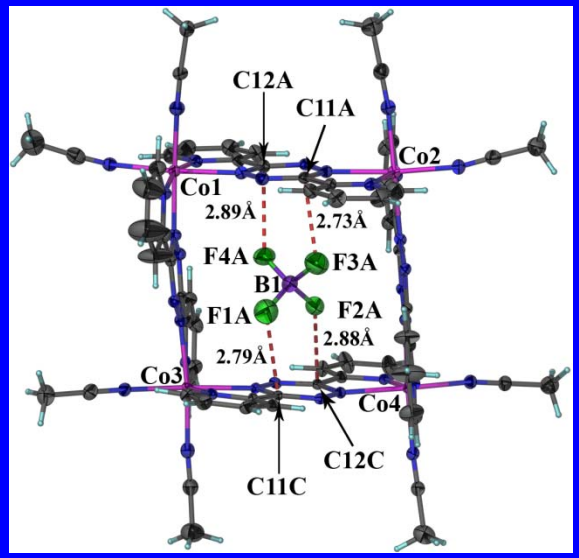


bppn

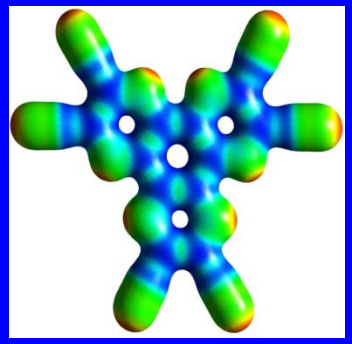


$[Ag_4(bppn)_4][SbF_6]_4$

- The different π-acidity of the central 3,6-bis(2´-pyridyl)-1,2,4,5-tetrazine (bptz) or 3,6-bis(2´-pyridyl)-1,2-pyridazine (bppn) rings affects the outcome of the reactions with $AgSbF_6$; reactions with bptz lead to propeller-type species $Ag_2(bptz)_3[SbF_6]_2$, whereas the bppn reactions produce the grid-type structure $[Ag_4(bppn)_4][SbF_6]_2$.
- Single crystal X-ray diffraction studies revealed that $[Co_4(NCCH_3)_8(bptz)_4{\subset}BF_4][BF_4]_7$ adopts the square motif with an encapsulated $[BF_4]^-$ anion, which is positioned so that the fluorine atoms of $[BF_4]^-$ are pointing to the electron deficient carbon atoms of two bptz ligands.

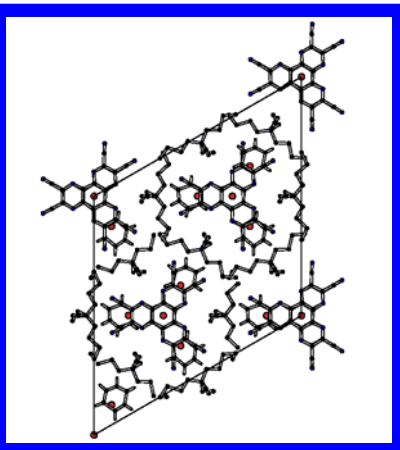


Cation of $[Co_4(NCCH_3)_8(bptz)_4{\subset}BF_4][BF_4]_7$



ESP map of electron-deficient hexaazatriphenylene hexacarbonitrile ($HAT(CN)_6$).

$[Br]^-$



Structure of $\{([n\text{-}Bu_4N][Br])_3[HAT(CN)_6]_2\}$.