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Hirshfeld Surface Analysis

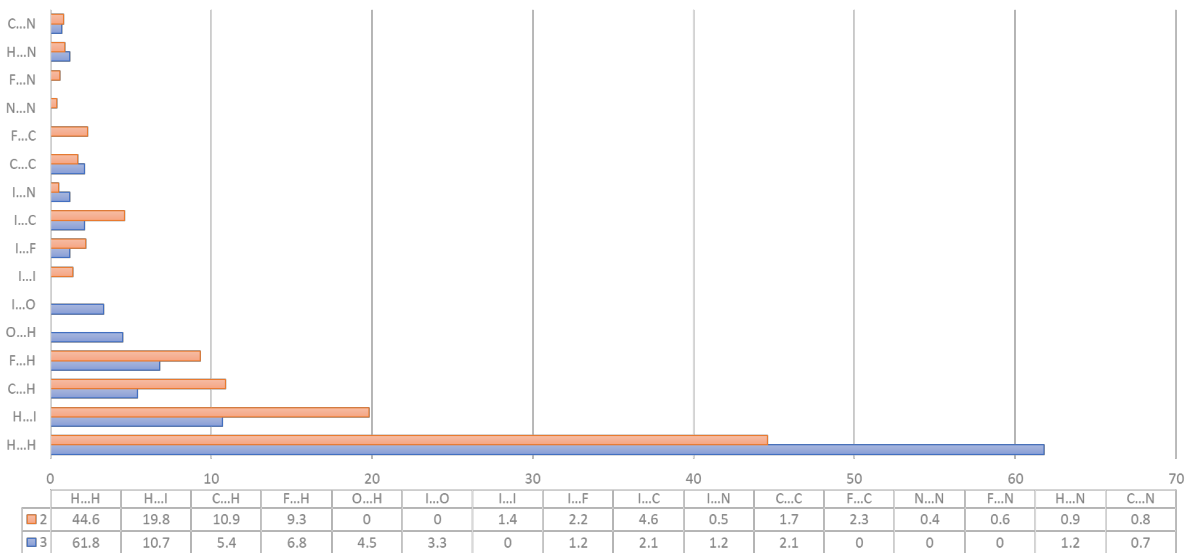
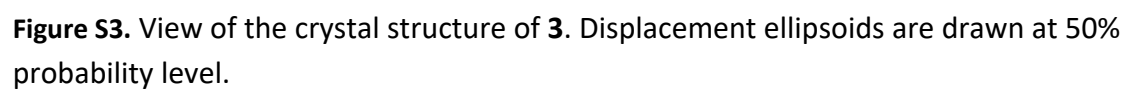
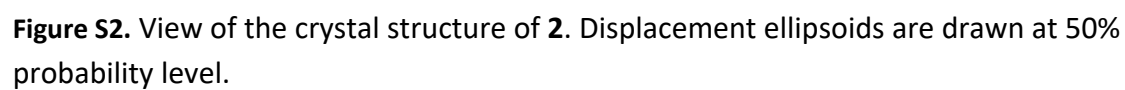


Figure S1. Percentage contributions of various intermolecular contacts to the Hirshfeld surface area in **2** and **3**.



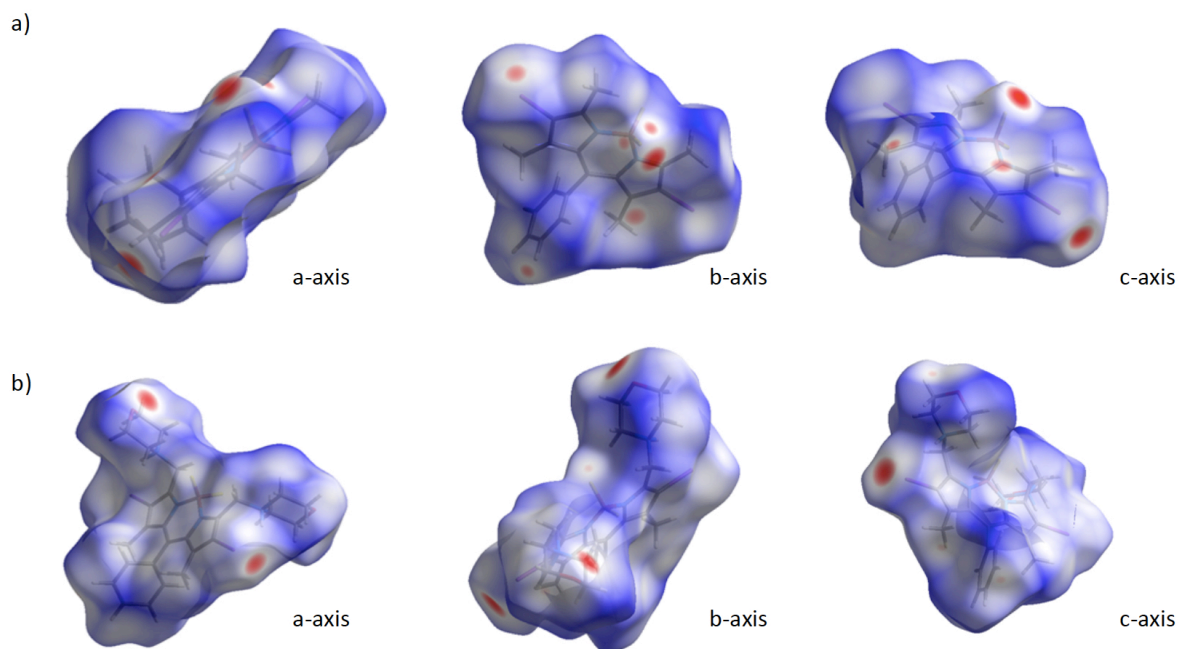


Figure S4. Views of the d_{norm} surfaces of a) **2** and b) **3**, viewed along different crystallographic axes.

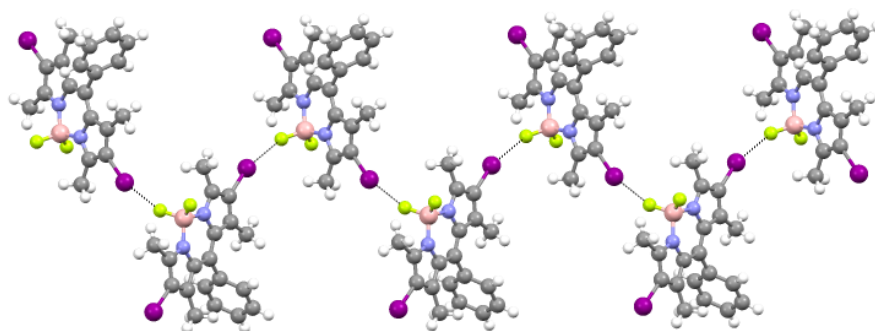


Figure S5. Chains observed in **2**, (polymorph I) formed by intermolecular C-I...F interactions.



Figure S6. Chains observed in polymorph II of ,6-diiodo-1,3,5,7-tetramethyl-8-phenyl-4,4-difluoroboradiazaindacene³⁵ formed by intermolecular C-I...I interactions.

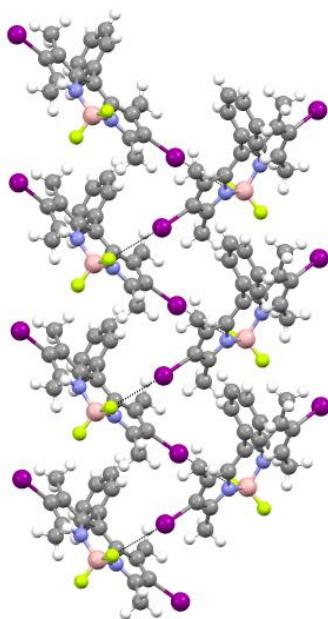


Figure S7. Chains observed in polymorph III of ,6-diiodo-1,3,5,7-tetramethyl-8-phenyl-4,4-difluoroboradiazaindacene³⁶ formed by intermolecular C–I⋯F interactions.

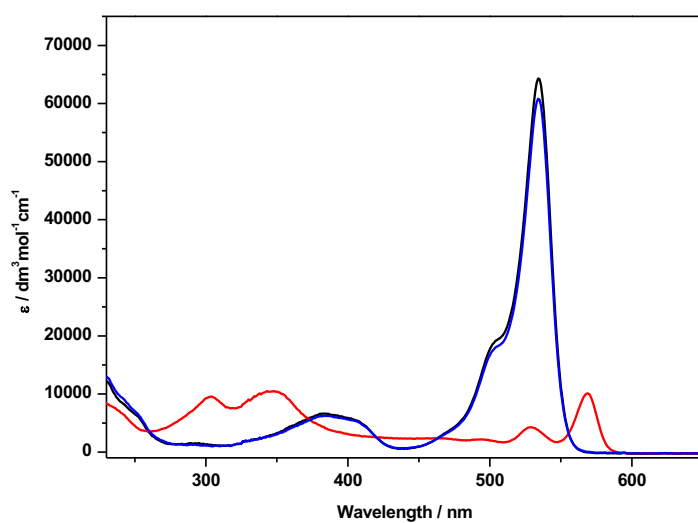


Figure S8. UV-vis spectroelectrochemistry of **2** in CH₂Cl₂ with [tBu₄N][BF₄] as electrolyte at 243 K. Black line is the spectral profile of **2** before reduction. Red line is the spectral profile of [2][−]. Blue line is the spectral profile obtained after the redox cycle.

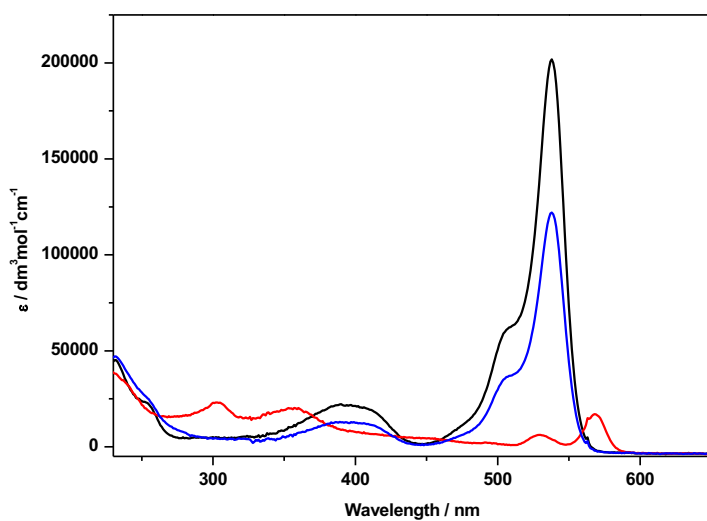


Figure S9. UV-vis spectroelectrochemistry of **3** in CH_2Cl_2 with $[\text{nBu}_4\text{N}][\text{BF}_4]$ as electrolyte at 243 K. Black line is the spectral profile of **3** before reduction. Red line is the spectral profile of $[\mathbf{3}]^-$. Blue line is the spectral profile obtained after the redox cycle.

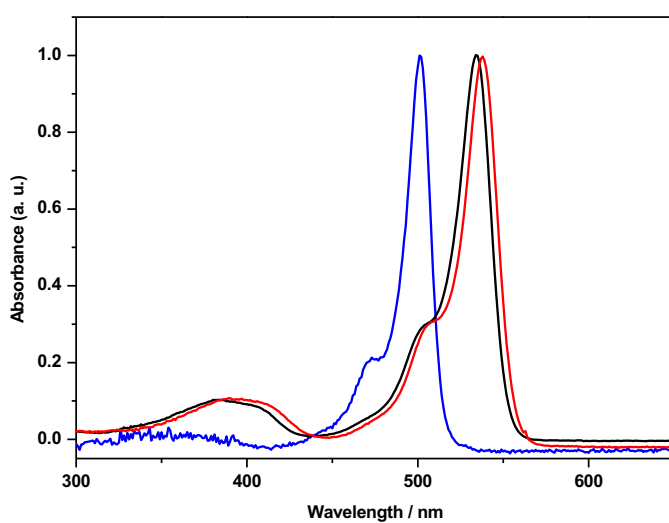


Figure S10. Normalized UV-vis absorption spectra of **1** (blue line), **2** (black line) and **3** (red line) in CH_2Cl_2 with $[\text{nBu}_4\text{N}][\text{BF}_4]$ as electrolyte at 243K.