

Supplimentary Information

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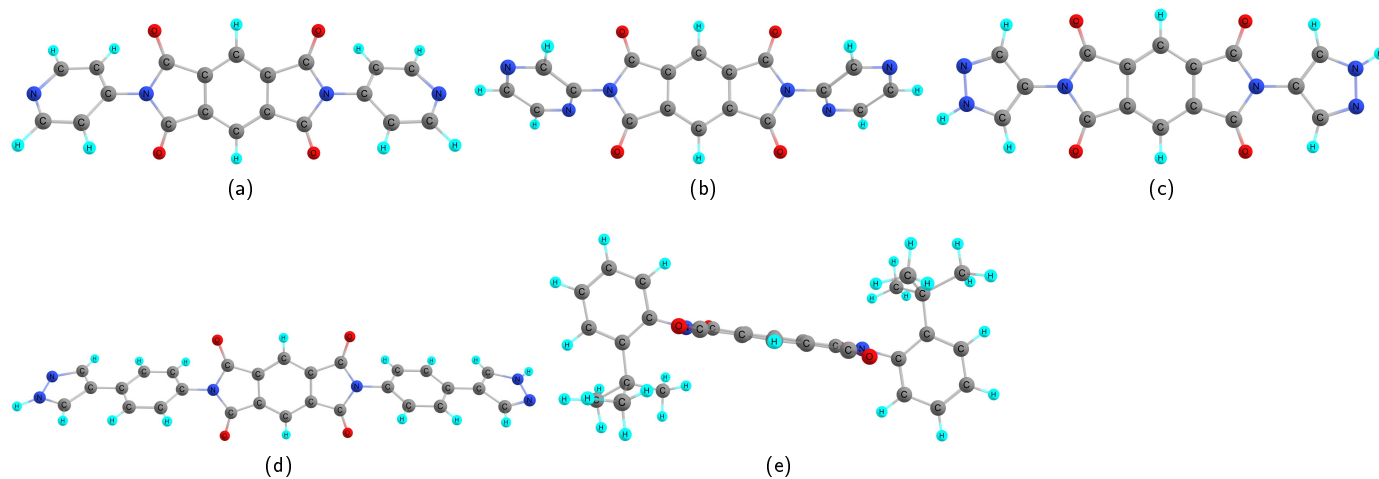


Figure S1: Optimized structures of pyromellitic diimide derivatives (a) BPyDI (b) BPyDI1 (c) BPIT (d) BPPIT and (e) BPPyDI.

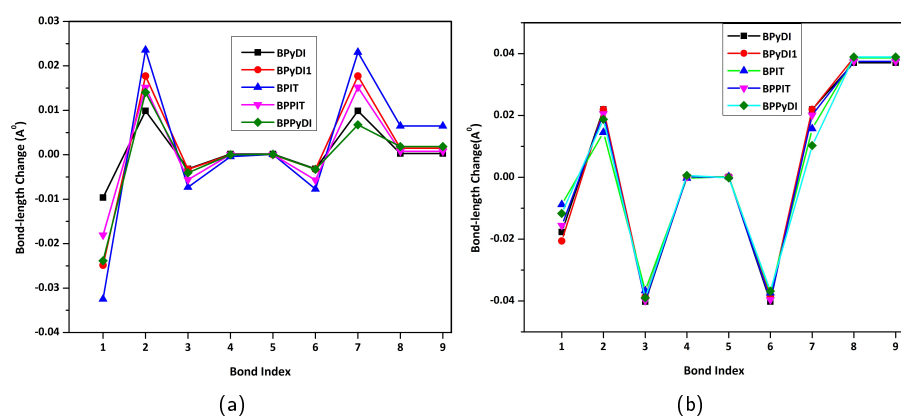


Figure S2: The change of bond length as a function of bond index of pyromellitic diimide derivatives; (a) oxidation (b) reduction.

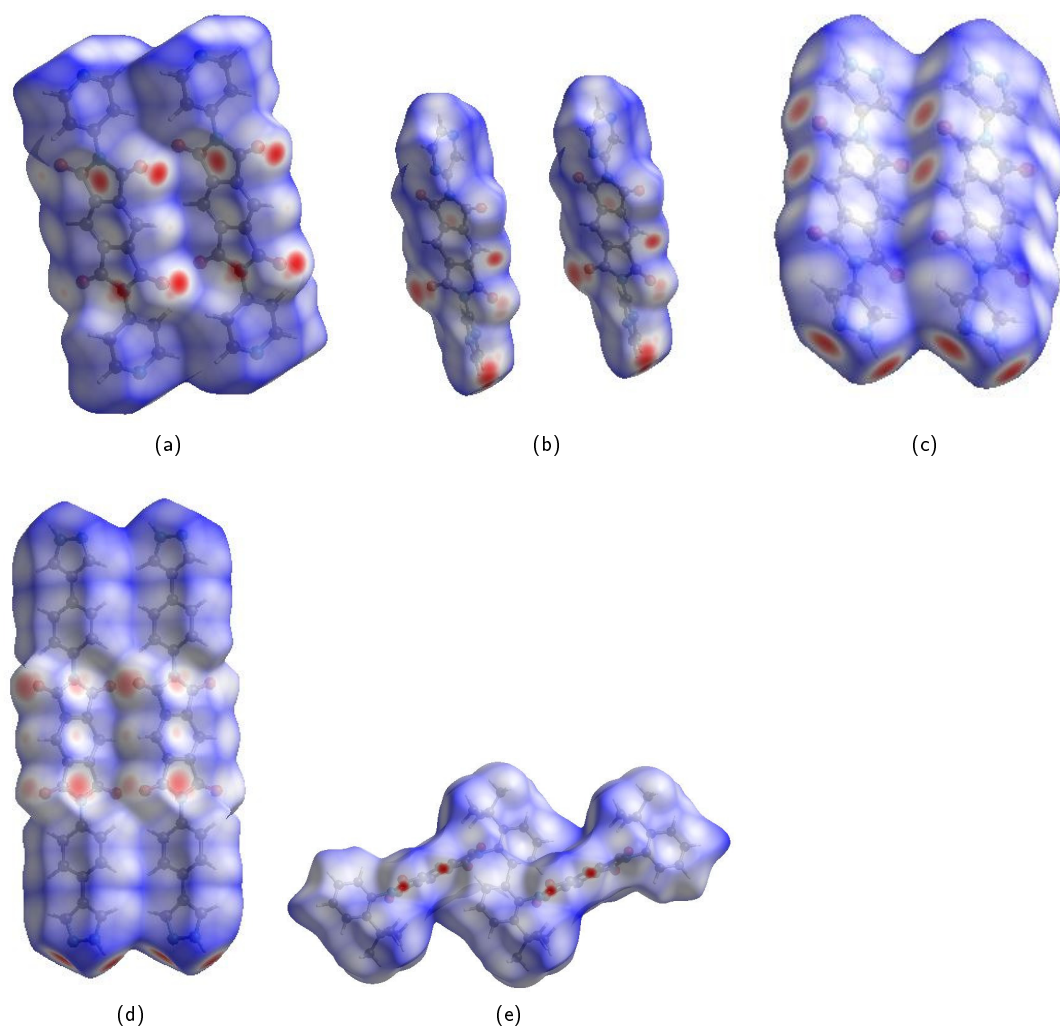


Figure S3: Hirshfeld Surface of the pyromellitic diimide derivatives; (a) BPyDI (b) BPyDI1 (c) BPIT (d) BBBIT and (e) BPPyDI.