Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Octathienyl/phenyl-substituted zinc phthalocyanines J-aggregated through conformational planarization

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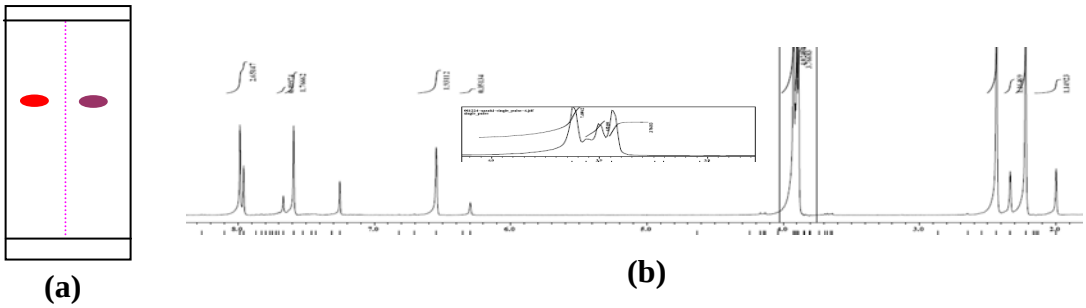
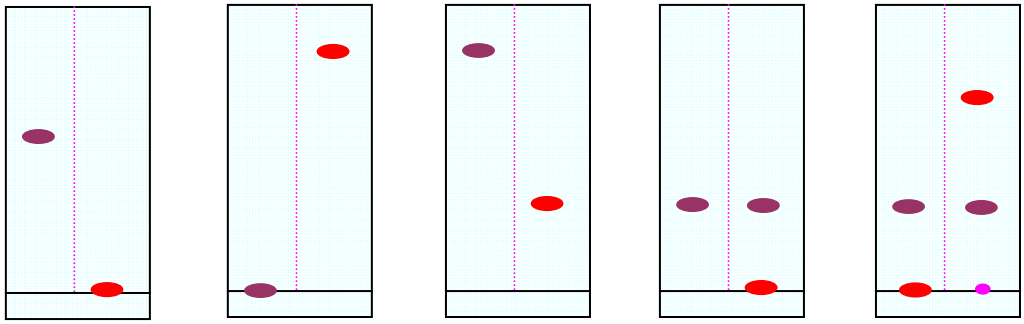


(a) **(b)**

Fig. S1 (a) The TLC experiment of 4,5-dibromophthalic acid dimethyl ester (left) and the product obtained from the Suzuki cross-coupling reaction (right), with a 2:1(volume ratio) mixed solvents of petroleum and ether ethyl acetate as the eluent. (b) ^{1}HNMR spectra of the product in $CDCl_3$.



(1) (2) (3) (4) (5)

Fig. S2 The TLC experiments in the synthesis of phthalonitrile 7 from the mixture obtained from the Suzuki cross-coupling reaction. In each TLC experiment, the left is reagent and the right is the product. (1) 2→3; (2) 3→4; (3) 4→5; (4) 5→6; (5) 6→7; The eluent is a 2:1(volume ratio) mixed solvents of petroleum and ether ethyl acetate.

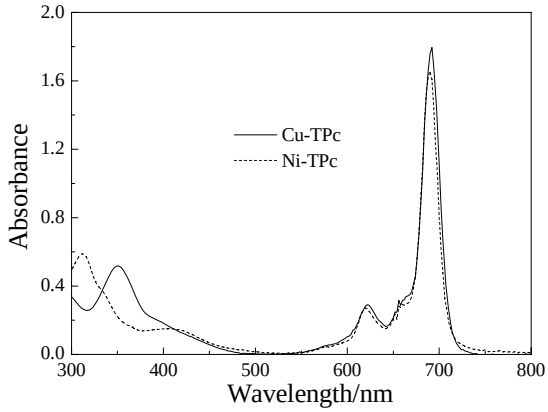


Fig. S3 The UV-Vis spectrum of Cu-TPc and Ni-TPc in THF (c = 1 ×10^{-4} mol. L^{-1}).
The sample is placed in a standard 1-mm quartz curvette

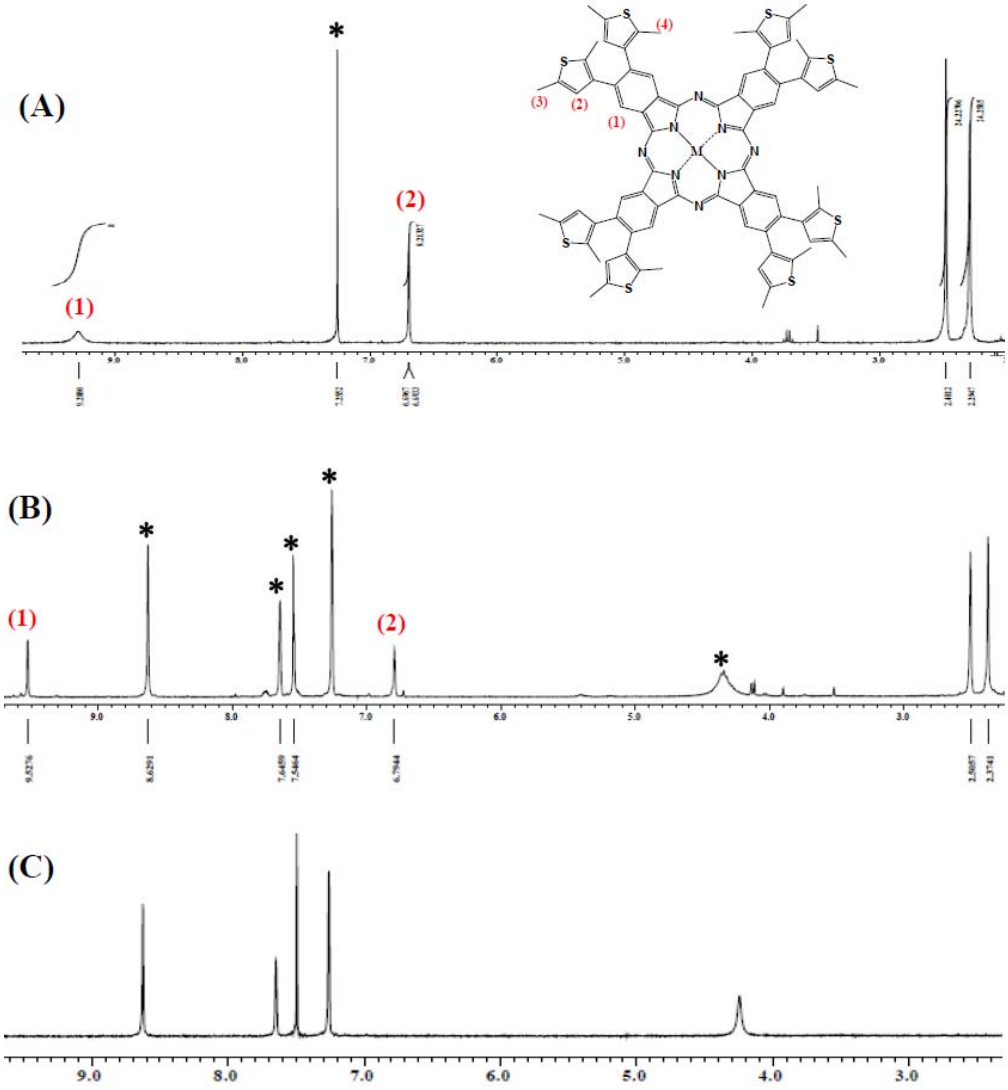


Fig. S4 ^{1}HNMR spectra of (A) Ni-TPc (1.5×10^{-3} mol.L^{-1}) in $CDCl_3$; (B) Zn-TPc (1.5×10^{-3} mol.L^{-1}) in the 5:1 mixed solvents of $CDCl_3$ and d_5-pyridine; (C) 5:1 mixed solvents of $CDCl_3$ and d_5-pyridine

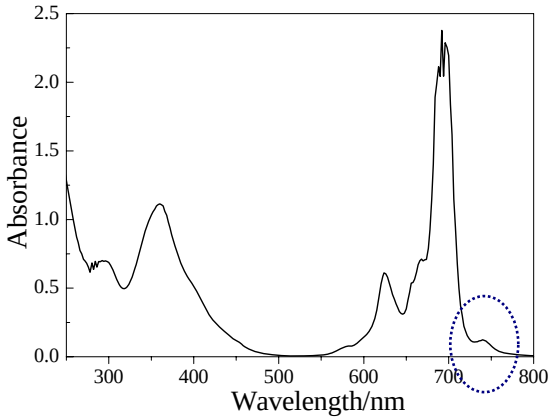


Fig. S5 The UV-Vis spectrum of Zn-TPc in THF (c = 2 ×10^{-5} mol. L^{-1})

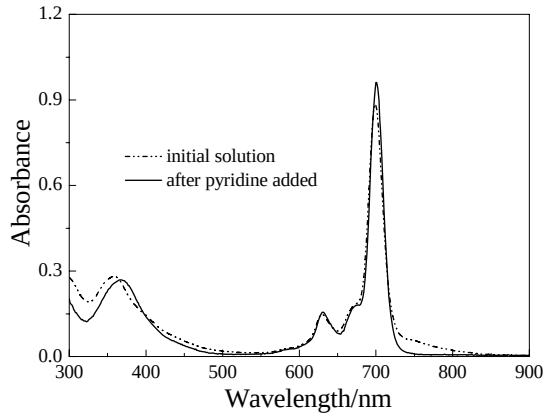


Fig. S6 The UV-Vis spectral changes of Zn-TPc (c = 2 ×10^{-5} mol. L^{-1}) in chloroform upon the addition of a drop of pyridine.

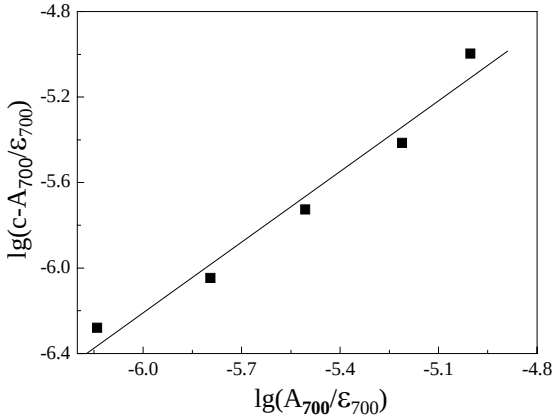


Fig. S7 The plot of lg(c-$A_{700}/\varepsilon_{700}$) versus lg($A_{700}/\varepsilon_{700}$) of Zn-TPc in the concentration range of 1.25 × 10^{-6} to 2 × 10^{-5} mol. L^{-1}.

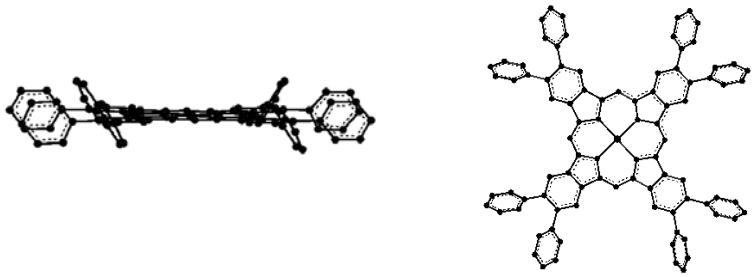


Fig. S8 Computer optimized conformation of Zn-PPc by energy minimization method. Left: side view; right: top view