Electronic Supplementary Material (ESI) for Dalton Transactions

Anionic 3D cage networks self-assembled by iodine and V-shaped pentaiodides using dimeric oxoammonium cations produced *in situ* as templates

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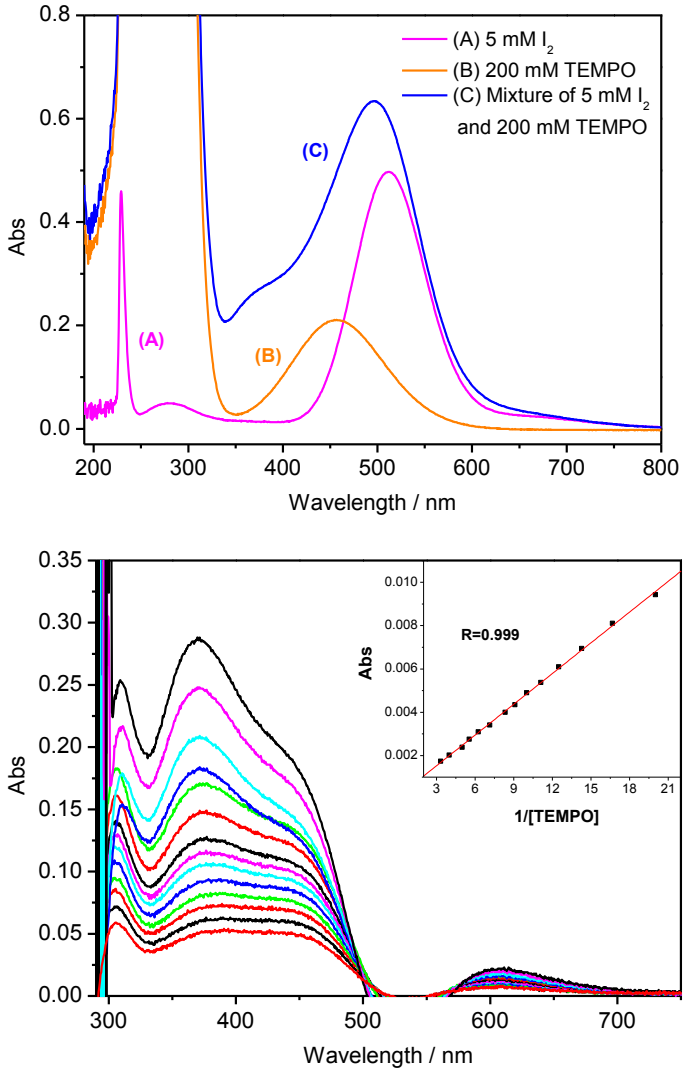

Fig. S1 (Up) UV-Vis absorption spectra of (A) 5 mM I_2, (B) 200 mM TEMPO, (C) mixture of 5 mM I_2 and 200 mM TEMPO in chloroform. (Down) Subtracted UV-Vis titration spectra to confirm the XB complex between I_2 and TEMPO in chloroform (inset line shows the double reciprocal Benesi-Hildebrand plot to obtain the stoichiometry, formation constant and extinction coefficient). K_{XBC} : 0.22 $M^{-1}$and ε_{XBC}: 2.73×10^3 $M^{-1}\cdot cm^{-1}$ in chloroform.

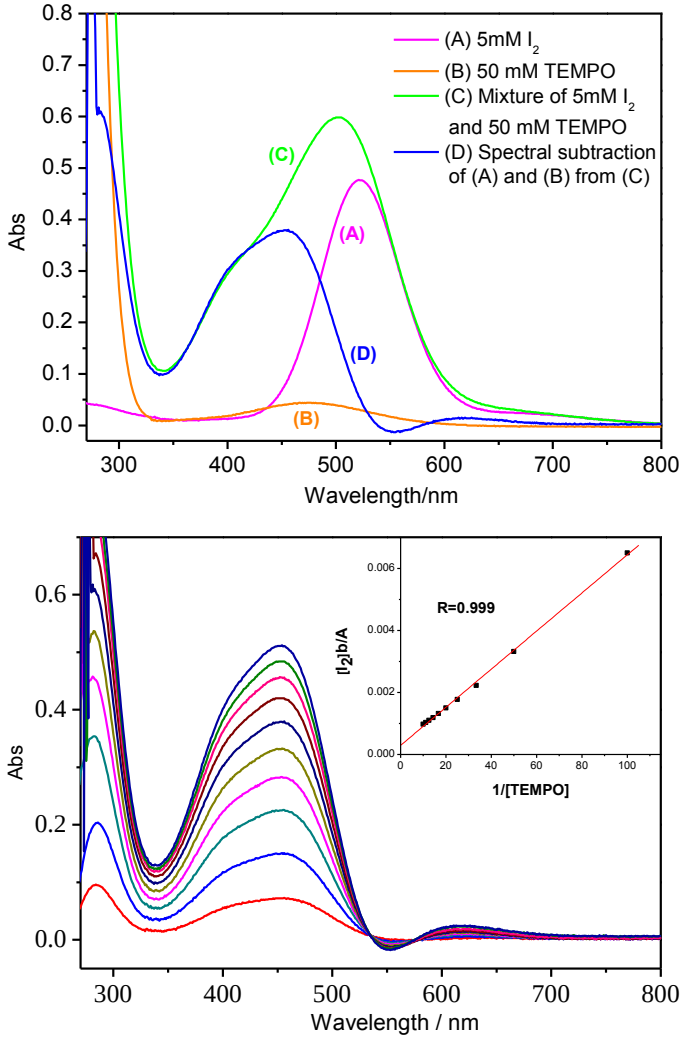

Fig. S2 (Up) UV-Vis absorption spectra of (A) 5 mM I_2, (B) 50 mM TEMPO, (C) mixture of 5 mM I_2 and 50 mM TEMPO, (D) spectral subtraction of (A) and (B) from (C) in *n*-hexane. (Down) Subtracted UV titration spectra to confirm the XB complex between I_2 and TEMPO in *n*-hexane (inset line shows the double reciprocal Benesi-Hildebrand plot to obtain the stoichiometry, formation constant and extinction coefficient). K_{XBC} : 4.8 M^{-1} and ε_{XBC}: 2.92×10^3 $M^{-1}\cdot cm^{-1}$ in *n*-hexane.

Scheme S1. Possible reaction processes for some relevant fragments.