

## Supporting information

### A mixed-valence $Mn_6$ cluster exhibiting self-assembled vesicular structure and catecholase-like activity in solution state

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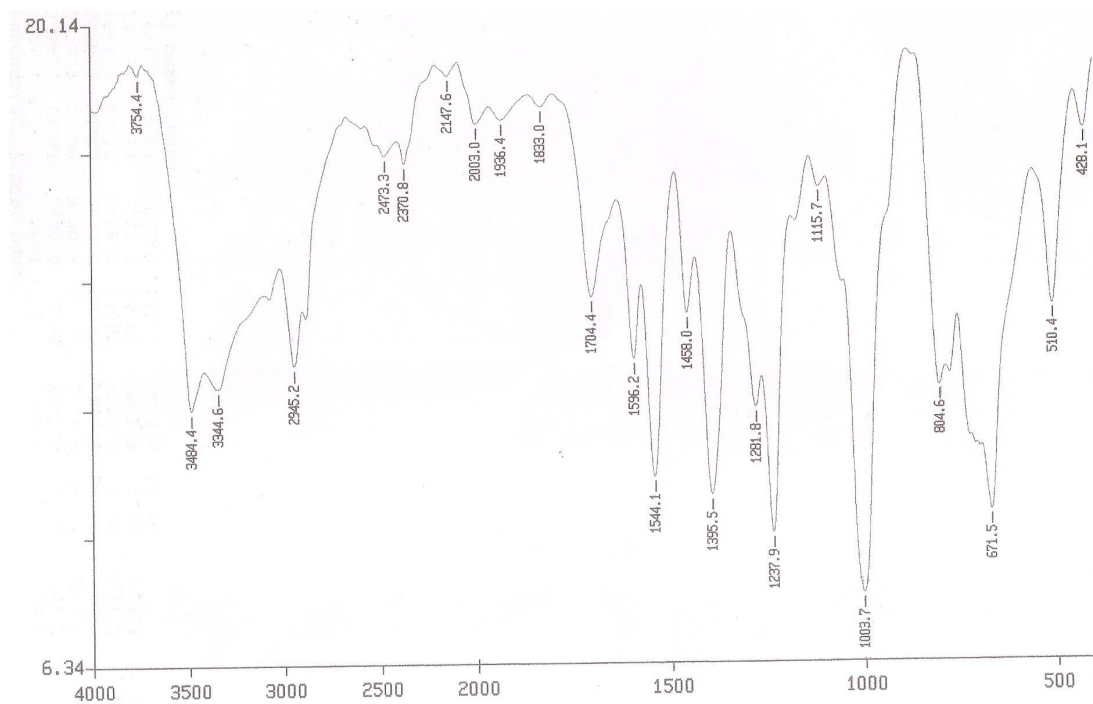
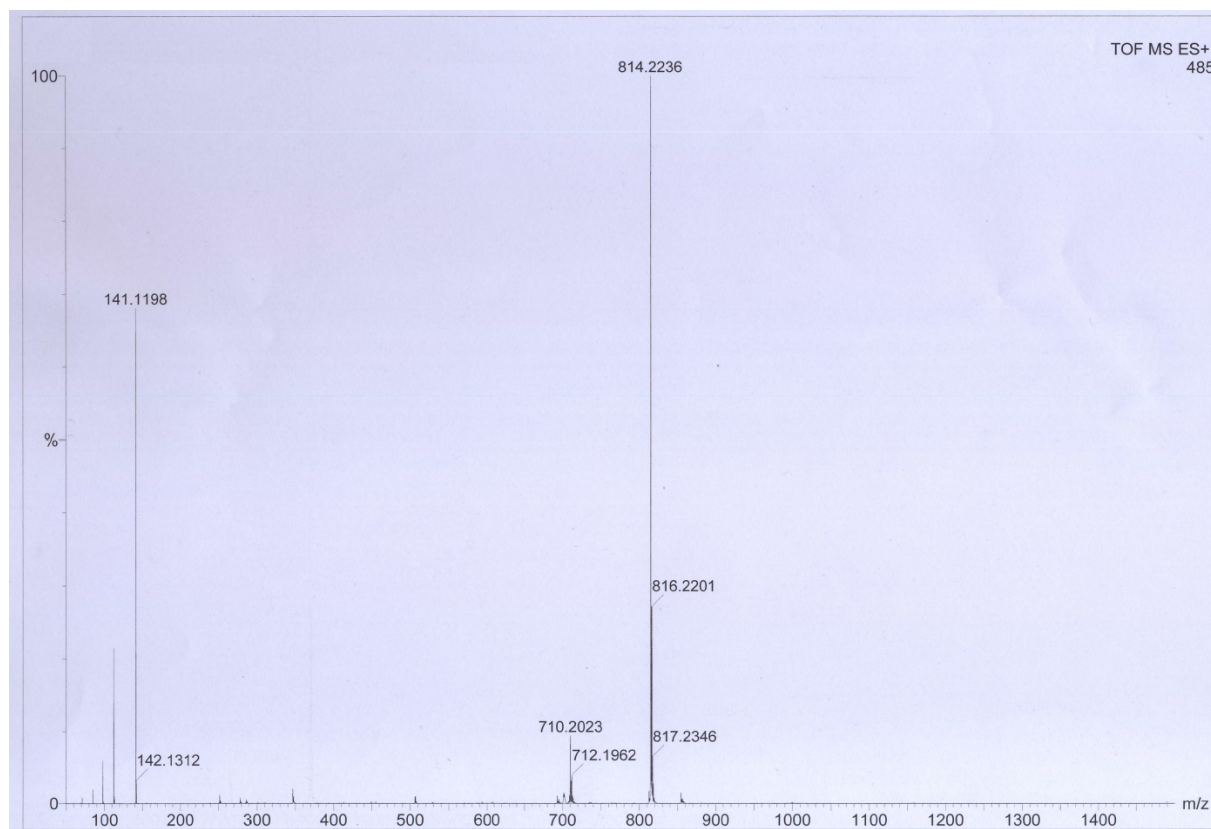
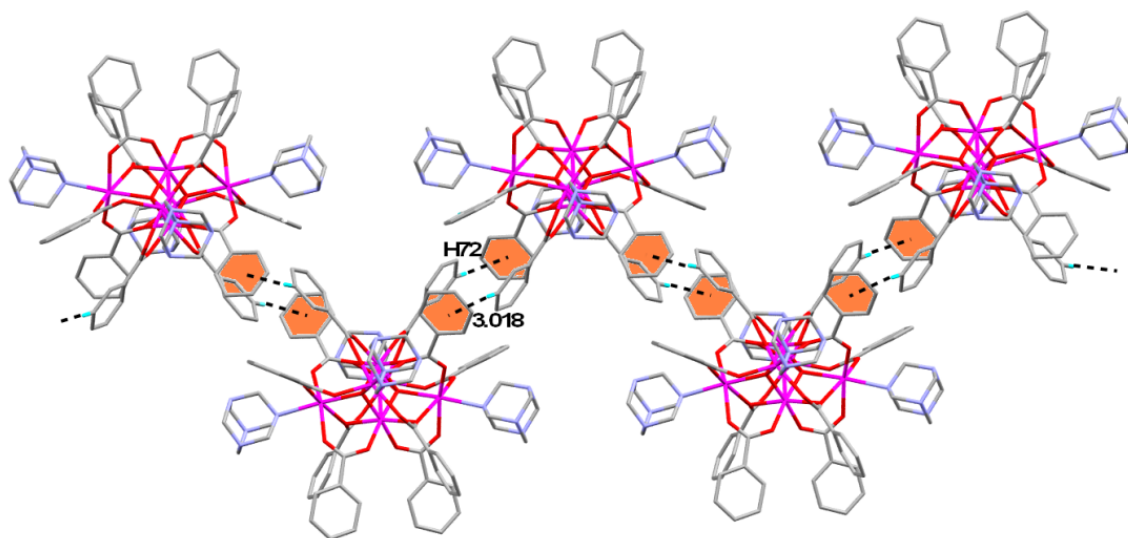


Figure S1. IR spectra of 1.

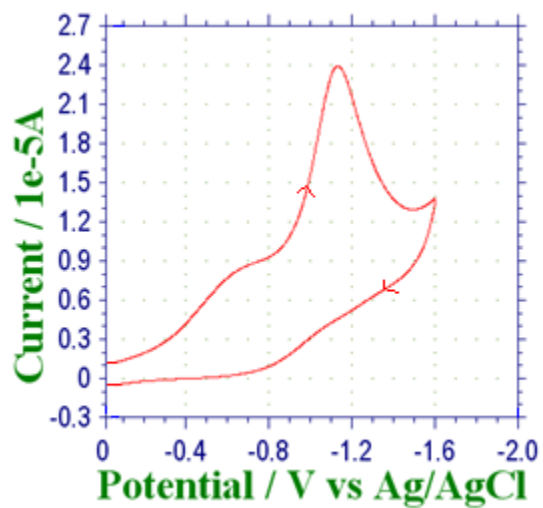


**Figure S2.** Electrospray ionization mass spectra (ESI-MS positive) of **1** in acetonitrile solvent.

In complex **1** there is no considerable  $\pi$ -stacking interaction between the aromatic rings. However, the complex is further stabilized by one C–H $\cdots$   $\pi$ (phenyl) interaction between the neighboring hexanuclear cores as shown in Figure S3. The distance between H72 and the Cg of the phenyl ring of an adjacent core is 3.018 Å and that between H72 and the nearest atom of the phenyl ring (C62) is 2.703 Å. C72–H72 $\cdots$ Cg angle being 165° (Cg = centroid of the phenyl ring).



**Figure S3.** C-H $\cdots$  $\pi$  supramolecular interaction in **1**.



**Figure S4.** The cyclic voltammogram of **1** in DMF solvent (scan rate  $0.1 \text{ V s}^{-1}$ ).