

Electronic supplementary information (ESI†)

Semi-insulating behaviour of self-assembled tin(IV)corrole nanospheres

Woormileela Sinha,^a Mohit Kumar,^b Antara Garai,^a Chandra Shekhar Purohit,^a
Tapobrata Som ^{*b} and Sanjib Kar^{*a}

^aSchool of Chemical Sciences, National Institute of Science Education and Research (NISER), Bhubaneswar – 751005, India.
E-mail: sanjib@niser.ac.in

^bInstitute of Physics, Sachivalaya Marg, Bhubaneswar – 751005, India. E-mail: tsom@iopb.res.in

- Fig. S1** Electronic absorption spectrum of 10-(2,4,5-trimethoxyphenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **1B**, (green line) 5,10,15-tris(4-cyanophenyl) corrolato-tin(IV)-chloride, **2B**, (blue line) and 10-(4-bromophenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **3B**, (red line) (Color online) in dichloromethane.
- Fig. S2** ^{13}C NMR spectrum of 10-(4-bromophenyl)-5,15-bis(4-cyanophenyl) corrolato-tin(IV)-chloride, **3B**, in CDCl_3 .
- Fig. S3** ESI- MS spectrum of (a) 10-(2,4,5-Trimethoxyphenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **1B** (b) 5,10,15-tris(4-cyanophenyl) corrolato-tin(IV)-chloride, **2B** and (c) 10-(4-bromophenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **3B** in CH_3CN shows the measured spectrum with isotopic distribution pattern.
- Fig. S4** ^1H NMR spectrum of 10-(2,4,5-Trimethoxyphenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **1B** in CDCl_3 .
- Fig. S5** ^1H NMR spectrum of 5,10,15-tris(4-cyanophenyl)corrolato-tin(IV) chloride, **2B** in CDCl_3 .
- Fig. S6** ^1H NMR spectrum of 10-(4-bromophenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **3B**, in CDCl_3 .
- Fig. S7** Single-crystal X-ray structure of 10-(2,4,5-Trimethoxyphenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **1B**, (a) top view (b) side view. Hydrogen atoms are omitted for clarity.
- Fig. S8** Single-crystal X-ray structure of 5,10,15-tris(4-cyanophenyl)corrolato-tin(IV) chloride, **2B**, (a) top view (b) side view, and (c) π - π stacking interactions. Hydrogen atoms are omitted for clarity.
- Fig. S9** Single-crystal X-ray structure of 10-(4-bromophenyl)-5,15-bis(4-cyanophenyl) corrolato-tin(IV)-chloride, **3B**, (a) top view (b) side view. Hydrogen atoms are omitted for clarity.
- Fig. S10** Vertical displacement of the peripheral carbon atoms from the N4 corrole planes in (a) **1B** (b) **2B** and (c) **3B**.

Fig. S11 EDX elemental analysis obtained from the nanospheres of **3B** showing the presence of the entire constituent elements: C, N, Cl, Br, and Sn.

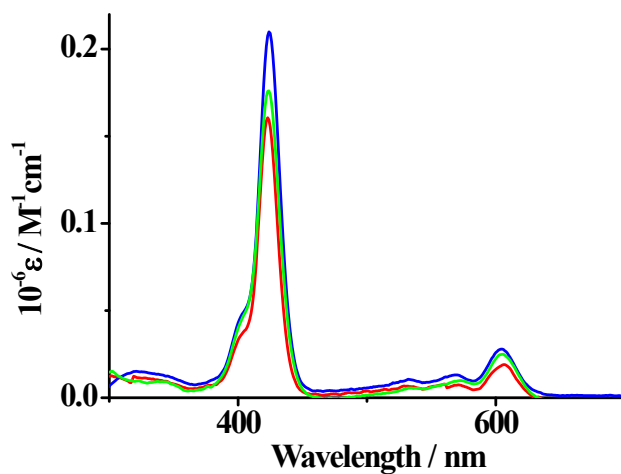


Fig. S1 Electronic absorption spectrum of 10-(2,4,5-trimethoxyphenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **1B**, (green line) 5,10,15-tris(4-cyanophenyl)corrolato-tin(IV)-chloride, **2B**, (blue line) and 10-(4-bromophenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **3B**, (red line) (Color online) in dichloromethane.

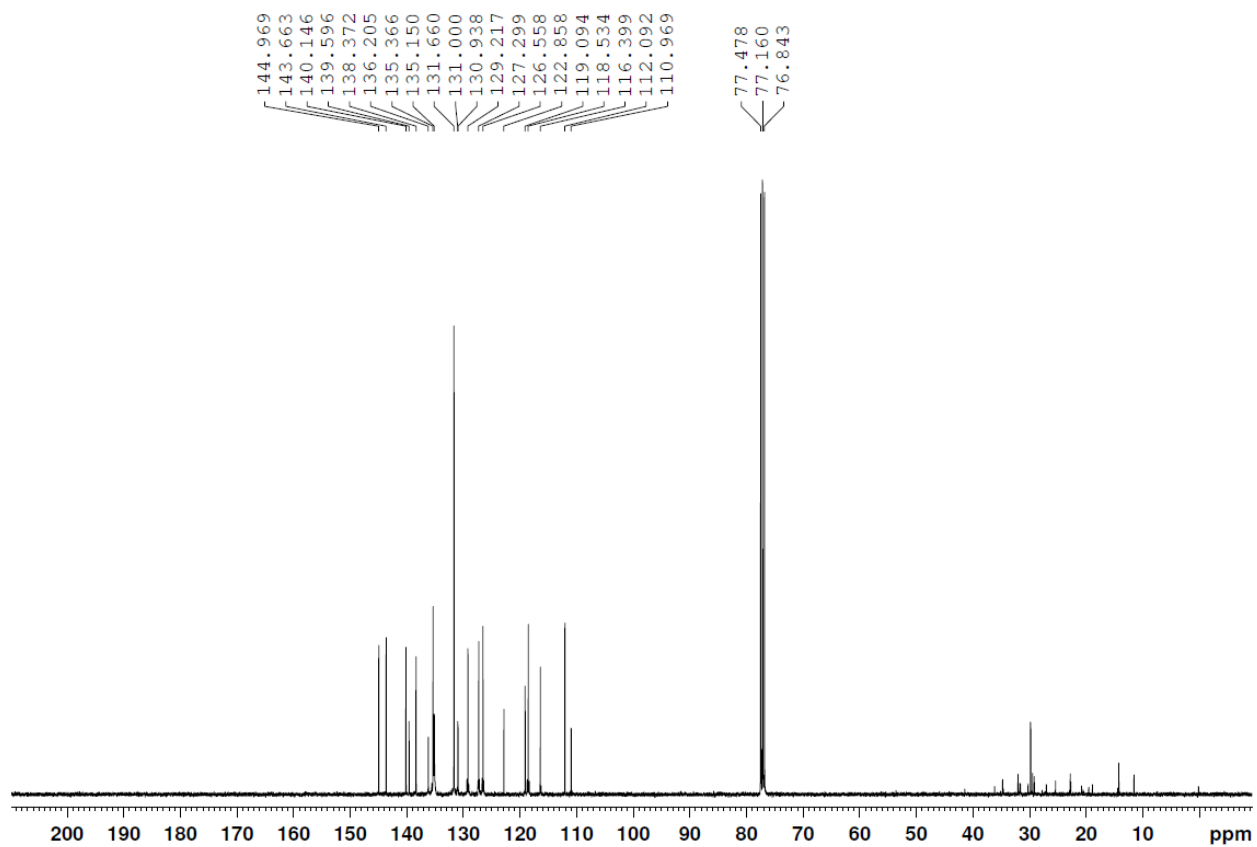


Fig. S2 ^{13}C NMR spectrum of 10-(4-bromophenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **3B**, in CDCl_3 .

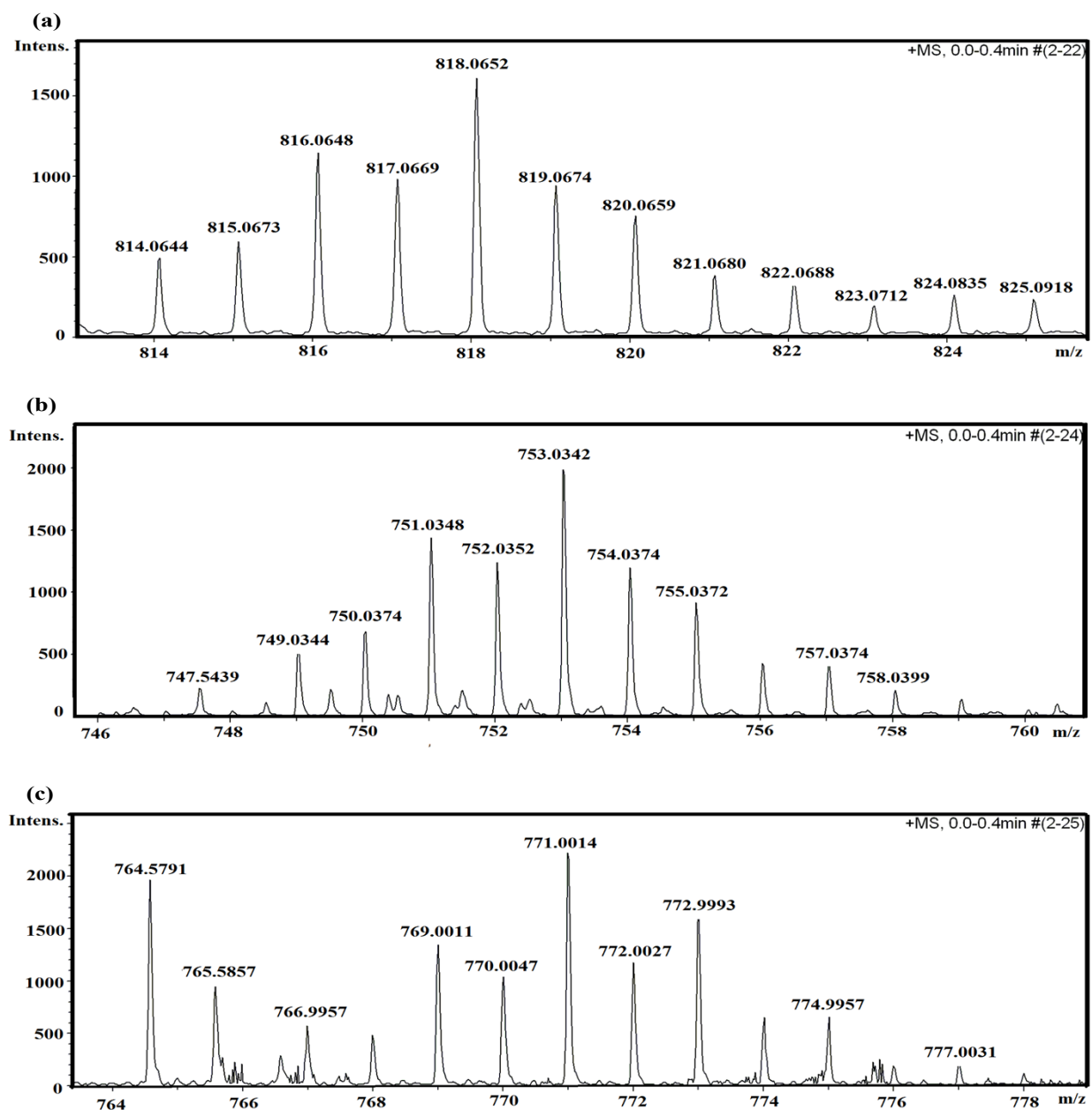


Fig. S3 ESI- MS spectrum of (a) 10-(2,4,5-Trimethoxyphenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **1B** (b) 5,10,15-tris(4-cyanophenyl)corrolato-tin(IV)-chloride, **2B** and (c) 10-(4-bromophenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **3B** in CH₃CN shows the measured spectrum with isotopic distribution pattern.

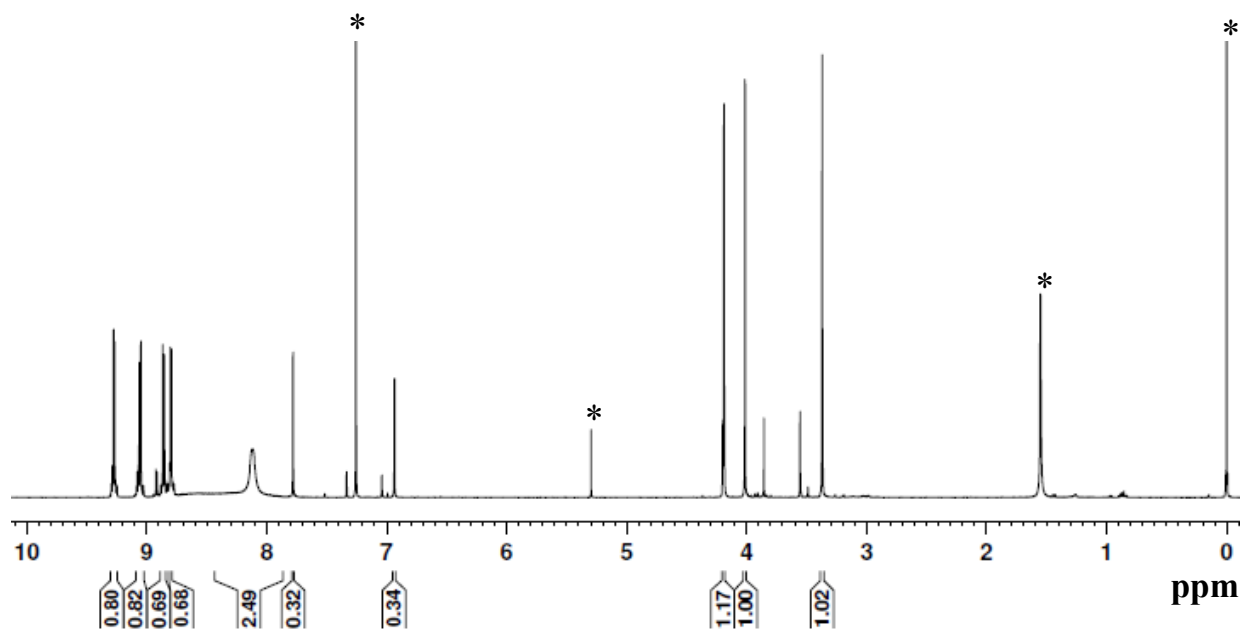


Fig. S4 ^1H NMR spectrum of 10-(2,4,5-Trimethoxyphenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **1B** in CDCl_3 .

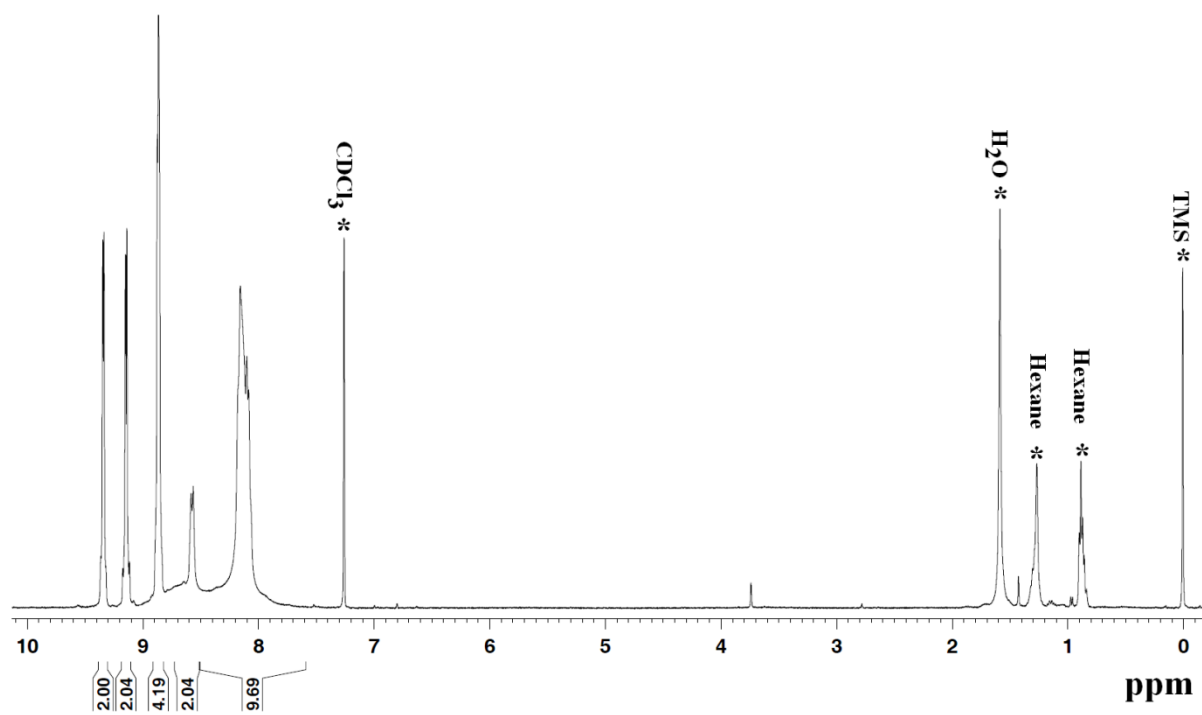


Fig. S5 ^1H NMR spectrum of 5,10,15-tris(4-cyanophenyl)corrolato-tin(IV)-chloride, **2B** in CDCl_3 .

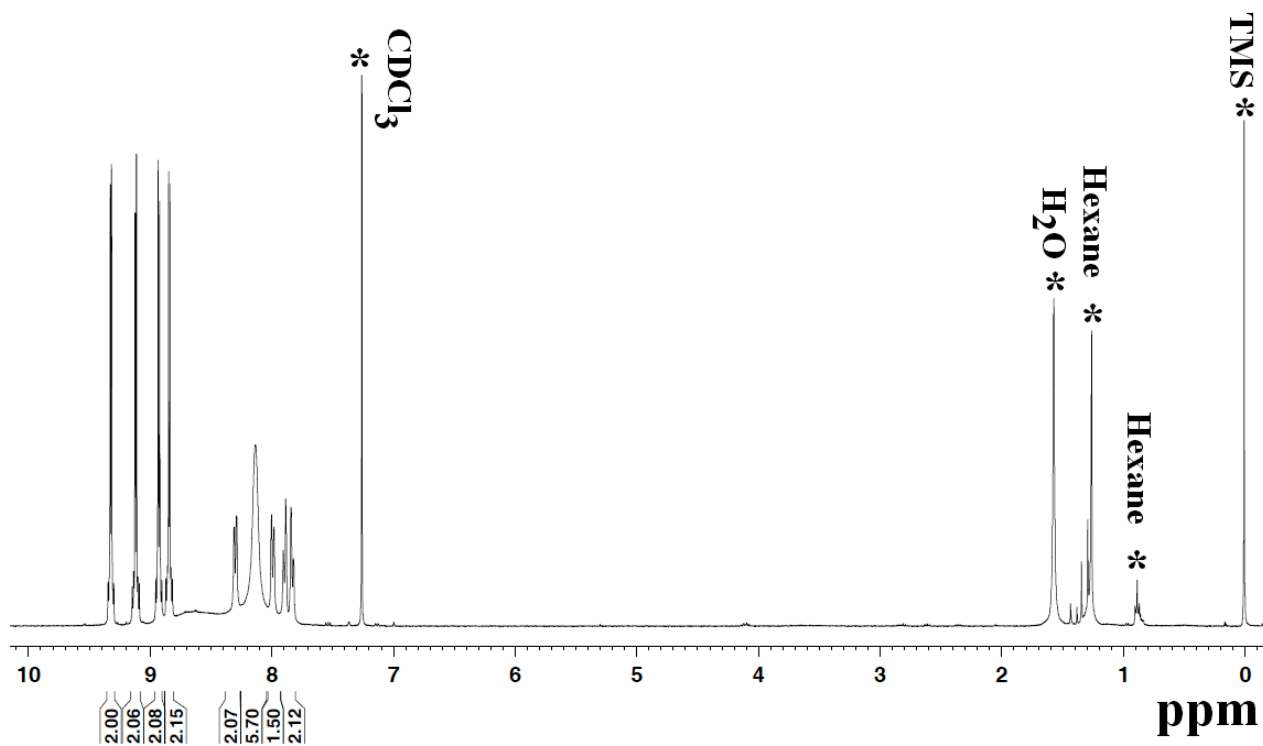


Fig. S6 ^1H NMR spectrum of 10-(4-bromophenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **3B**, in CDCl_3 .

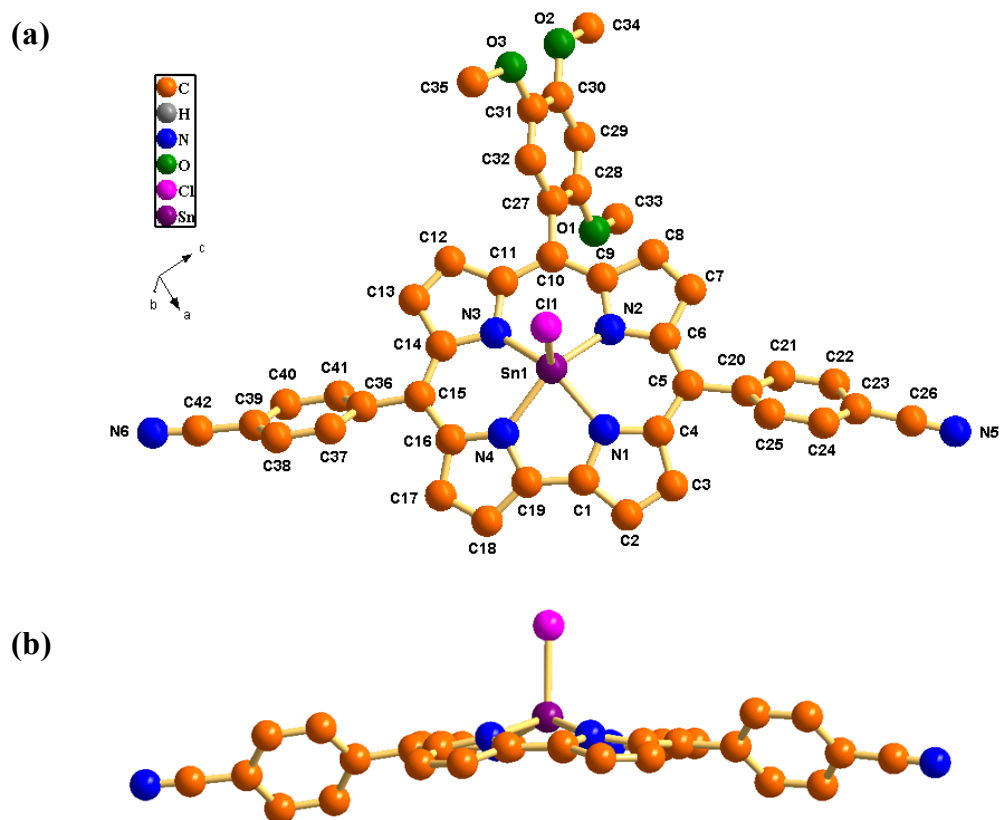


Fig. S7 Single-crystal X-ray structure of 10-(2,4,5-Trimethoxyphenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **1B**, (a) top view (b) side view. Hydrogen atoms are omitted for clarity.

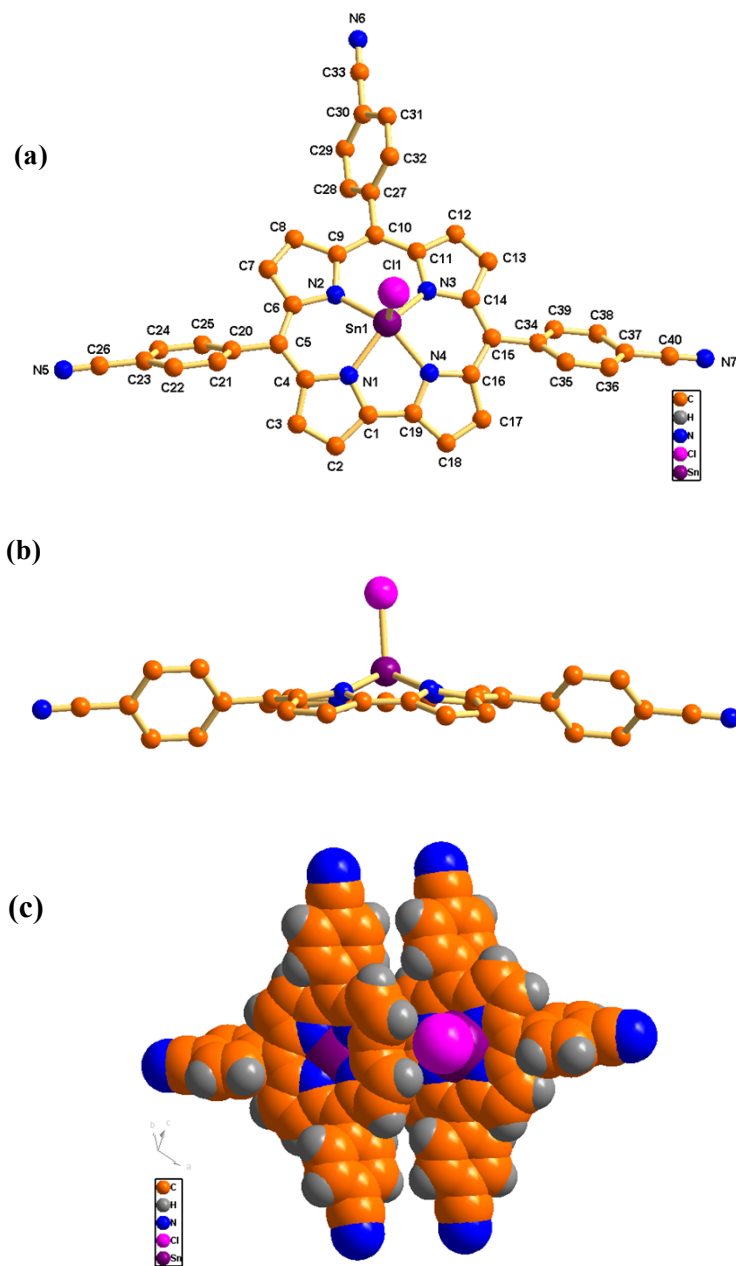


Fig. S8 Single-crystal X-ray structure of 5,10,15-tris(4-cyanophenyl)corrolato-tin(IV)-chloride, **2B**, (a) top view (b) side view, and (c) π - π stacking interactions. Hydrogen atoms are omitted for clarity.

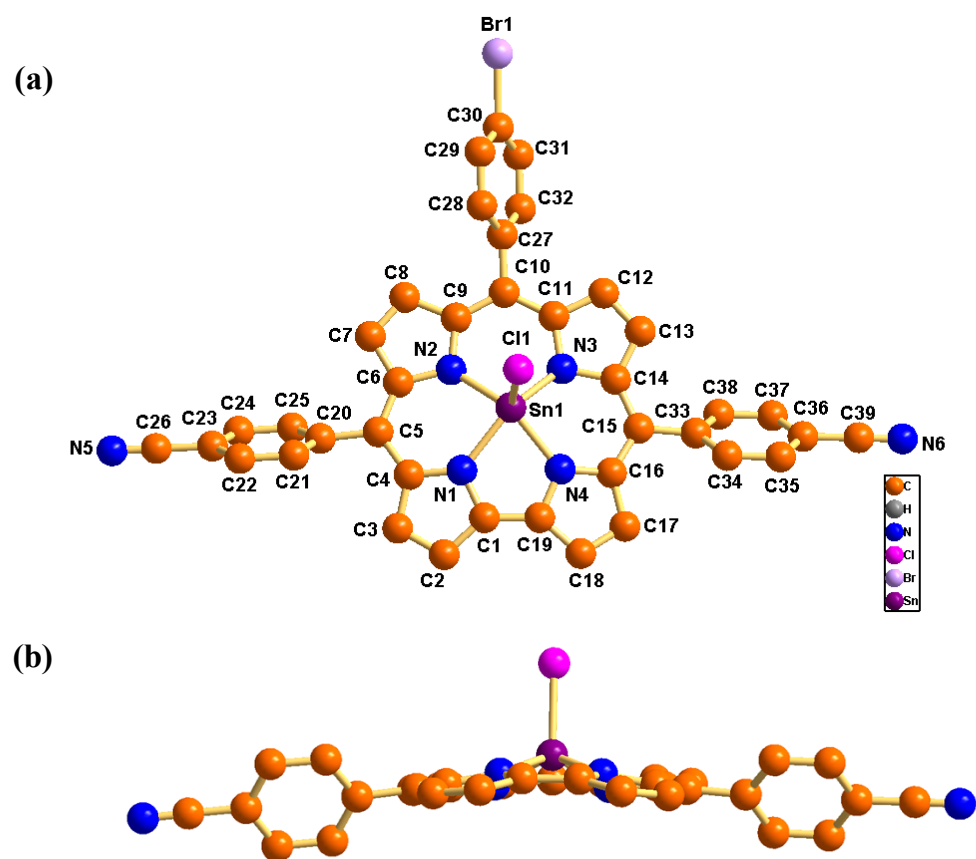


Fig. S9 Single-crystal X-ray structure of 10-(4-bromophenyl)-5,15-bis(4-cyanophenyl)corrolato-tin(IV)-chloride, **3B**, (a) top view (b) side view. Hydrogen atoms are omitted for clarity.

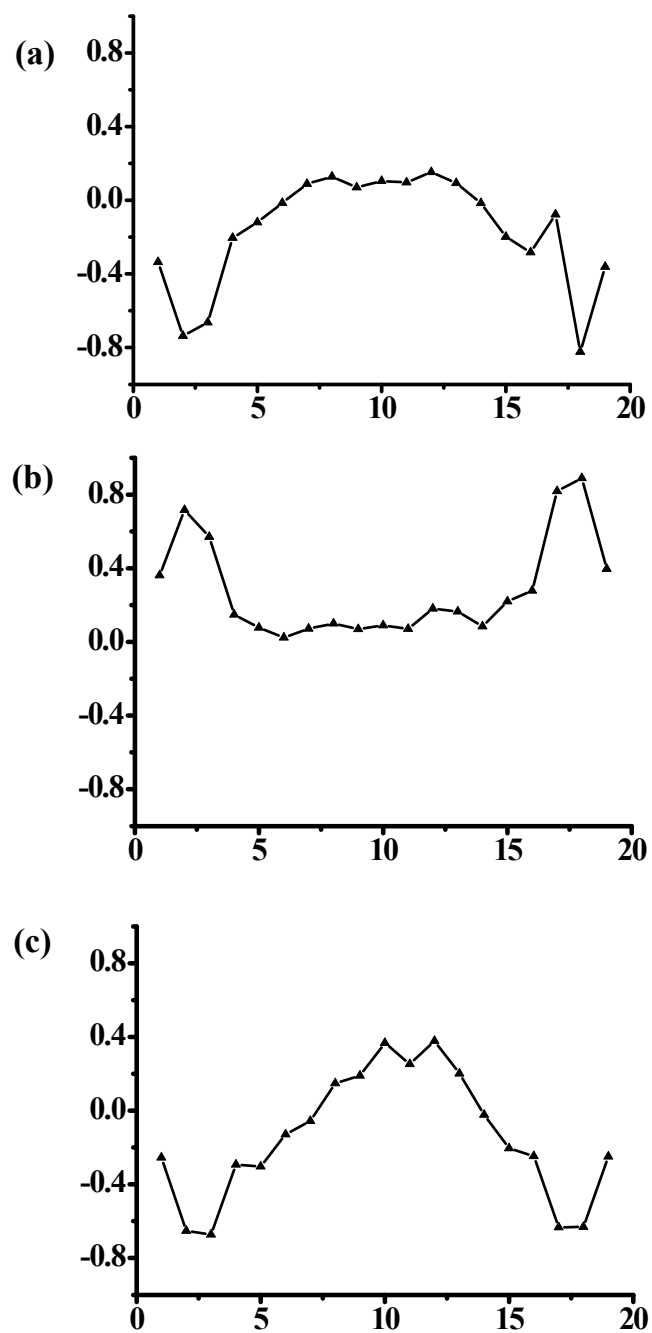
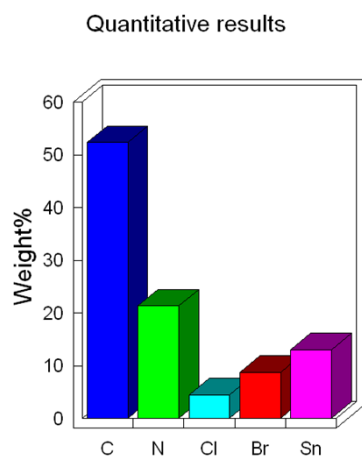
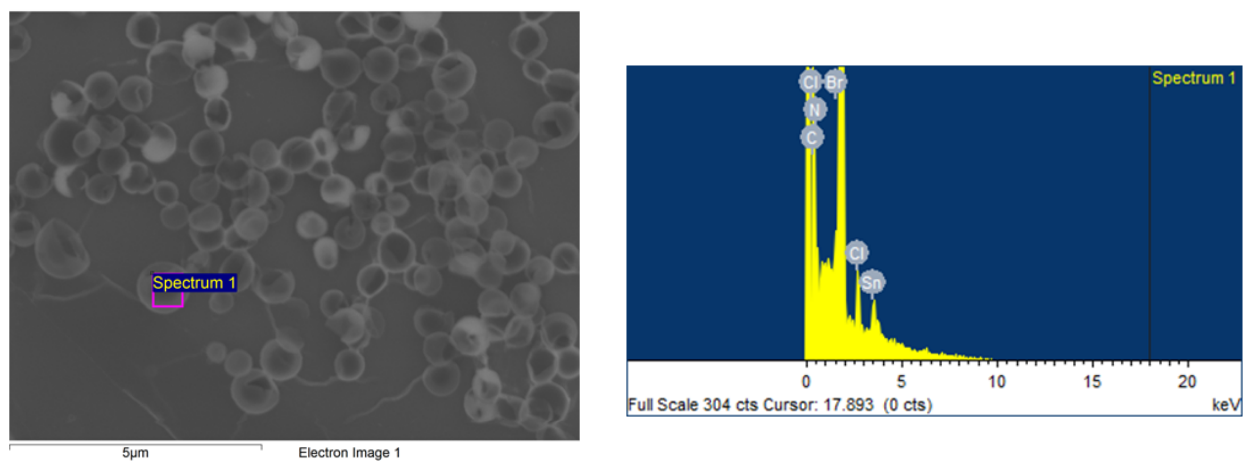


Fig. S10 Vertical displacement of the peripheral carbon atoms from the N4 corrole planes in (a) **1B** (b) **2B** and (c) **3B**.



Element	Weight%
C K	52.32
N K	21.35
Cl K	4.51
Br L	8.79
Sn L	13.03
Totals	100.00

Fig. S11 EDX elemental analysis obtained from the nanospheres of **3B** showing the presence of the entire constituent elements: C, N, Cl, Br, and Sn.