Intermolecular Tl…H-C anagostic interactions in luminescent pyridyl functionalized thallium (I) dithiocarbamates

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Electronic Supplementary Material (ESI)

Table S1. Selected bond lengths (Å) and angles (°) for complexes.

Bond Distances	1	2	3	4
Tl(1)—N(36)$3	2.980(12)	2.921(13)	2.934(7)	2.919(6)
Tl(1)—S(13)	2.961(4)	2.976(4)	3.008(2)	3.021(2)
Tl(1)—S(11)	3.051(3)	3.054(3)	3.072(2)	3.054(2)
Tl(1)—S(13)$1	3.218(4)	3.212(4)	3.234(2)	3.191(2)
Tl(1)—S(11)$1	3.333(3)	3.387(3)	3.269(2)	3.283(2)
Tl(1) —S(13)$2	3.500(4)	3.478(3)	3.431(2)	3.356(2)
Tl(1)—Tl(1)$1	3.771(2)	3.817(12)	3.763(1)	3.735(1)
Bond angles				
S(13)—Tl(1)—S(11)	58.75(9)	58.83(8)	57.98(5)	58.41(4)
S(13)—Tl(1)—S(13)$1	104.92(9)	103.92(8)	105.94(4)	106.14(4)
S(11)—Tl(1)—S(11)$1	107.75(8)	107.51(7)	107.25(4)	107.88(4)
S(11)—Tl(1)—S(13)$1	81.08(9)	81.13(8)	80.98(5)	81.65(4)
N(36)$3—T(l)— S(13)$1	156.8(3)	157.0(3)	155.89(16)	154.37(13)
N(36)$3—Tl(1)—S(11)	85.5(3)	85.1(3)	85.76(15)	83.23(13)
N(36)$3—Tl(1)—S(13)$2	77.9(3)	79.5(3)	79.97(14)	83.27(13)
N(36)$3—Tl(1)—S(11)$1	149.6(3)	149.5(3)	150.15(16)	150.89(13)
N(36)$3-Tl(1)-S(13)	83.8(3)	84.2(2)	79.97(14)	82.99(11)
S(13)-Tl(1)-S(11)$1	80.51(9)	79.41(8)	81.36(5)	80.64(4)
S(11)$1 - Tl(1) - S(13)$1	53.50(8)	53.27(8)	53.90(5)	54.48(4)
S(13)$1 - Tl(1) - S(13)$2	101.41(6)	101.69(5)	100.07(3)	99.24(3)
S(11)$1 - Tl(1) - S(13)$2	103.70(8)	101.49(8)	100.30(5)	97.59(4)
S(11) - Tl(1) - S(13)$2	141.85(9)	145.01(8)	145.83(5)	148.52(5)
S(13) - Tl(1) - S(13)$2	149.53(6)	148.09(6)	148.35(3)	146.73(3)
N(36)$3- Tl(1) - Tl(1)$1	134.3(2)	134.1(2)	133.86(4)	132.19(4)
S(13)-Tl(1) - Tl(1)$1	55.56(8)	54.75(7)	55.71(4)	55.16(4)
S(11) - Tl(1) - Tl(1)$1	57.33(6)	57.78(7)	56.05(4)	56.78(5)
S(13)$1- Tl(1) - Tl(1)$1	49.36(8)	49.17(7)	50.23(4)	50.98(4)
S(11)$1 - Tl(1) - Tl(1)$1	50.42(6)	49.73(6)	51.21(3)	51.10(4)
S(13)$2-Tl(1) - Tl(1)$1	147.75(7)	146.32(7)	146.16(4)	144.43(5)

Symmetry elements in **1** and **2** $1 1-x, -y, 1-z $2 1/2+x, 1/2-y, 1-z; $3 1/2-x, 1/2+y, z;

In **3** $1 -x, 2-y, 1-z, $2 -x, y+1/2, 1/2-z $3 x, 3/2-y, z-1/2

In **4** $1 1-x, 1-y, 1-z $2 1/2-x, 1/2+y, 1-z, $3 x-1/2, 1/2-y, z

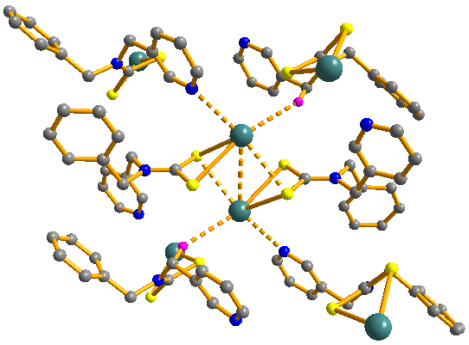
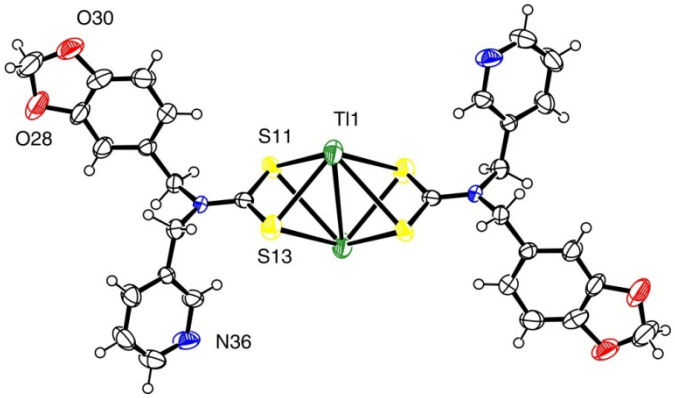
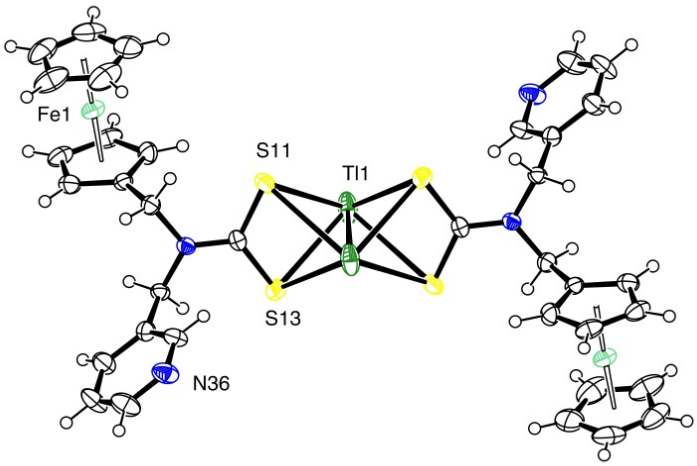


Fig. S3 2-D polymeric structure of **1** through interactions within the dimers.



(3)



(4)

Fig. S4 The dimeric structures of **3** and **4** with ellipsoids shown at 30% probability.

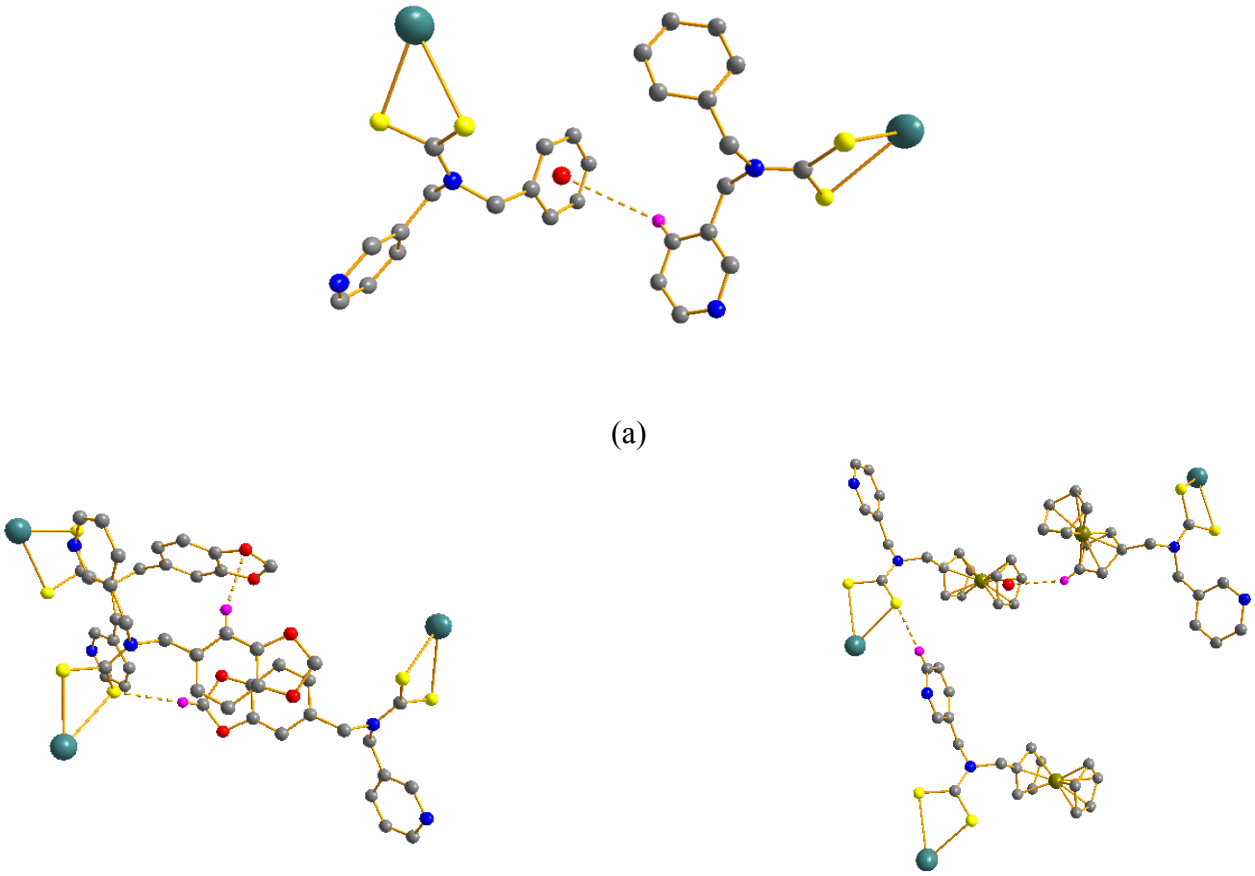


Fig. S5 (a) Supramolecular structure sustained through C-H...π in **1**. **2** is isomorphous (b) C-H…S and C-H…O interactions in **3** and (c) C-H...π and C-H…S interactions in **4**.

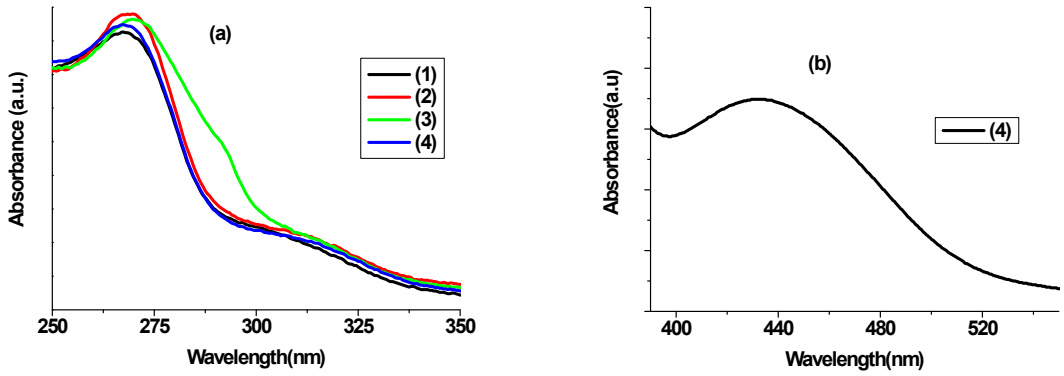


Fig. S6 (a) Electronic absorption spectra of **1-4** in solution (b) for **4** an additional band at low energy.

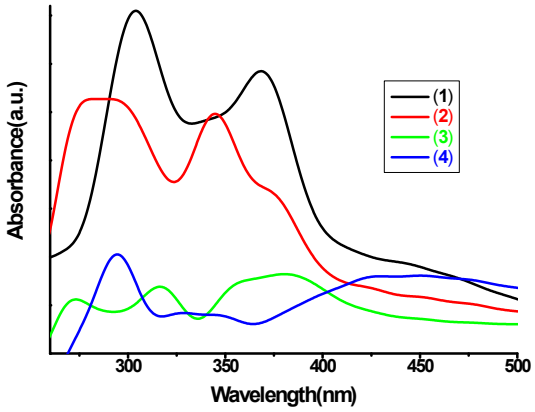


Fig. S7 Solid phase (nujol mull) UV-Vis. spectra of **1-4.**

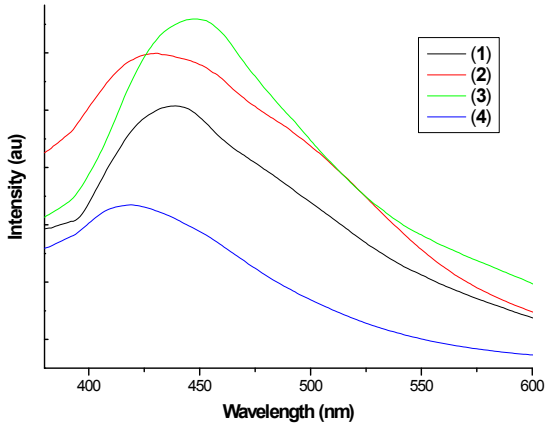


Fig. S8 Photoluminescence spectra in solid state (**1-4**).

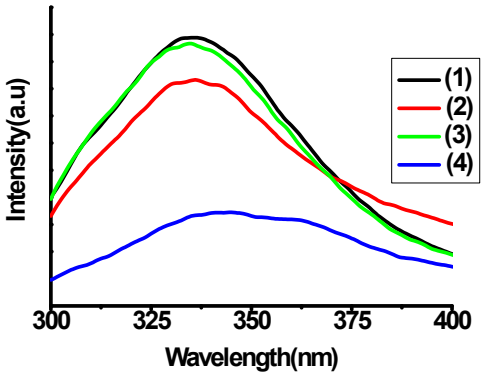


Fig. S9 Excitation and emission spectra of **1-4** at λ_{ex} = 300 nm in solution.