

Polymorphism and photoluminescence in naphthalene-based ligand, and its supramolecular structures through second - sphere coordination with $[\text{CoCl}_4]^{2-}$ anion^{†‡}

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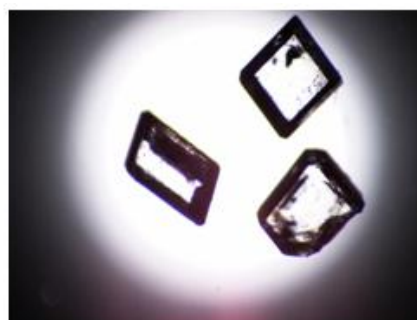
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Table S1. Crystallization of L1 in different conditions.

Solvents	Conditions	Form
Dichloromethane + ethanol	hexanedioic acid	α (a large amount) + β (a small amount)
Dichloromethane + ethanol	5% boric acid	α (a large amount) + β (a small amount)
Dichloromethane + ethanol	+5% boric acid + 10% NaClO_4	α
Dichloromethane + ethanol	Aniline	α
Dichloromethane + ethanol	Pyridine	α



(a)



(b)

Fig. S1 Crystal of two polymorphs: (a) α and (b) β

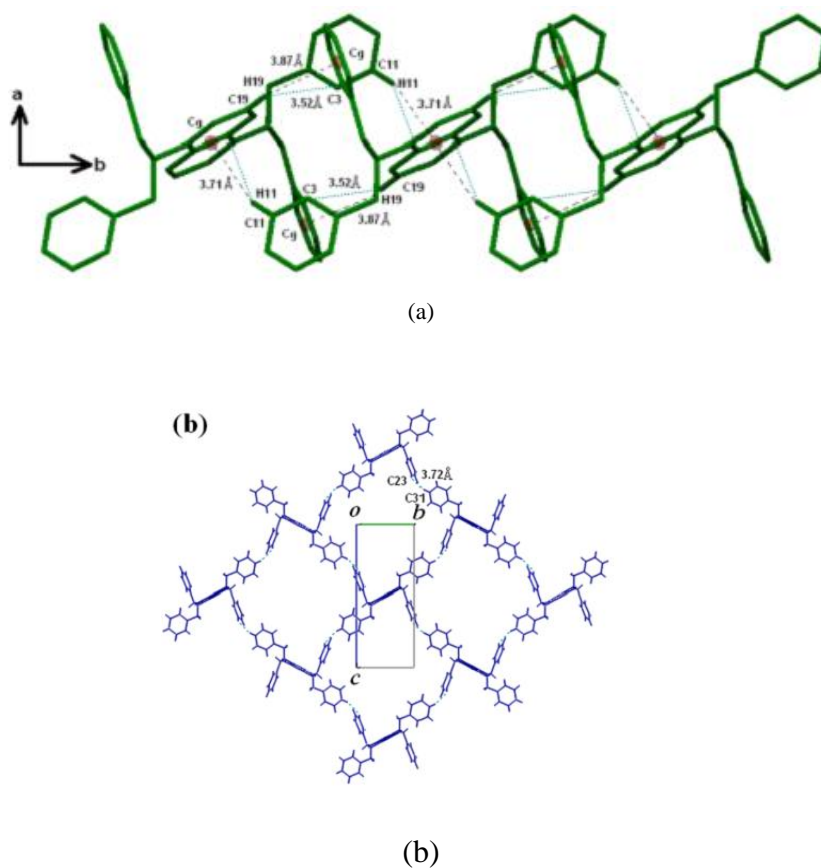


Fig.S2 (a) Two types of C-H... π interactions in molecule 1 of polymorph α , involving the aromatic rings of adjacent molecules; (b) Every four molecule 2 of polymorph α form a circled network involving extensive C-H... π interactions, and further extended into a layer along b-c plane.

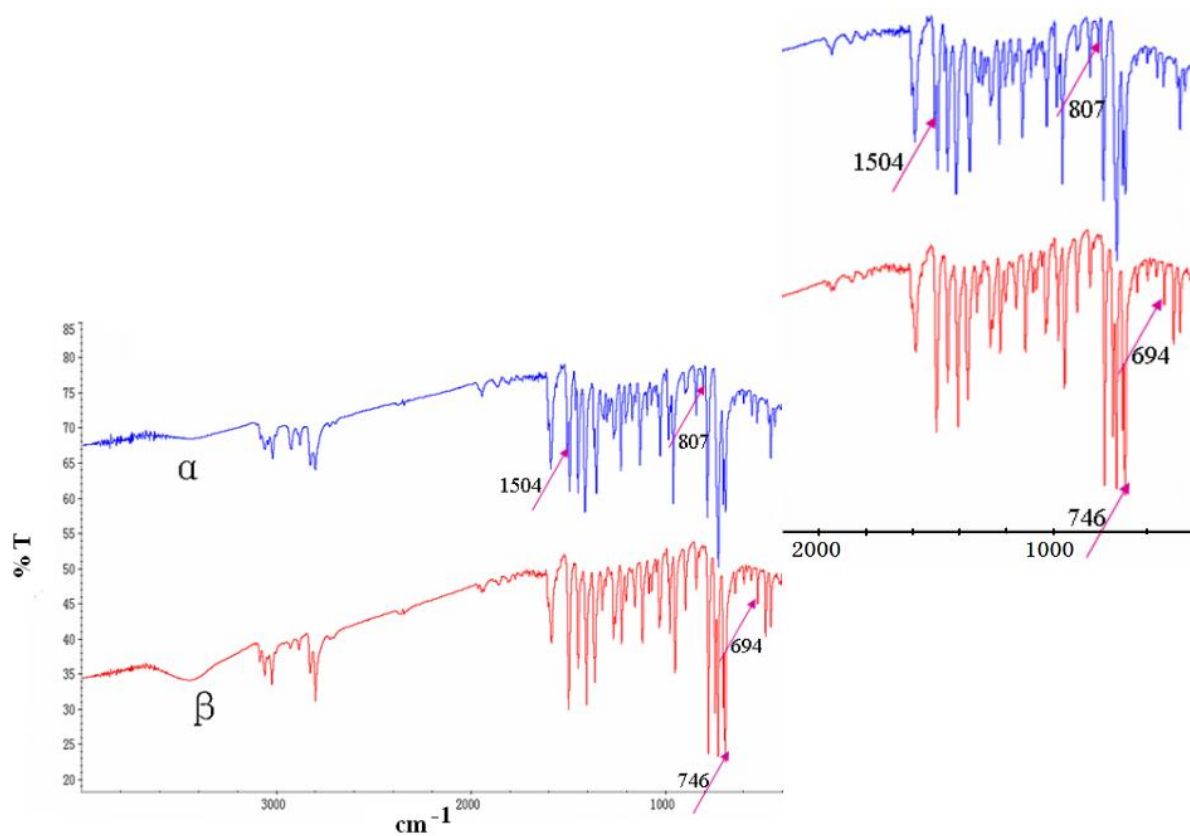


Fig. S3 IR spectra of the two polymorphs. The IR absorption bands 1350-1000 cm^{-1} are characteristic for the C-N stretching vibration. The absorption bands 1600-1450 cm^{-1} are assigned to C=C skeletal vibration of benzene and naphthalene. The absorption bands 3100-3000 cm^{-1} and 880-680 cm^{-1} are the stretching vibration and bending vibration of C-H of benzene and naphthalene. The absorption bands 2926-2800 cm^{-1} are assigned to C-H stretching vibration of $-\text{CH}_2$.

Table S2. Hydrogen bonding in the crystal structures of two polymorphs and the inclusion complexes.

	D...A(Å)	H...A (Å)	D-H...A (°)
β			
C8-H8...Cg(C9-C14)	3.491 (1)	2.647 (1)	143.2 (1)
(x,y,-1+z)			
C11-H11...C3 (1+x,y, -1+z)	3.518 (1)	2.785 (1)	134.5 (1)
α			
C19-H19...C3(1-x,1-y,1-z)	3.520 (1)	2.839 (1)	129.4 (1)
C11-H11...Cg(C15-C19)	3.717 (1)	2.812 (1)	159.6 (1)
(1-x,1-y,1-z)			
C20-H20B...C14	3.687 (1)	2.855 (1)	142.1(1)
(-x,1-y,1-z)			
Crystal 1			
C2-H2...Cg (C26-C31)	3.287(1)	2.644(1)	126.8(1)
N1-H1N...Cl2 (1+x,y,z)	3.183(1)	2.321(1)	158.1(1)
N2-H2N....Cl4 (x,y,z)	3.191(1)	2.315(1)	154.2(1)
(2-x, 1-y,-z)			
Crystal 2			
N1-H1...Cl1 (1-x, -y, -z)	3.252(1)	2.344(1)	147.4(1)
N2-H2...Cl2 (-x,1-y,1-z)	3.418(1)	2.562(1)	156.0(1)