



STRUCTURAL
CHEMISTRY

Volume 75 (2019)

Supporting information for article:

Killing two birds with one stone: 2D+2D→3D parallel stacking and 3D self-penetrating structures in one reaction and their crystal-to-crystal transformation

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Supporting information

Table S1 Selected geometric parameters (Å, °)

Complex 1			
Ni1-O3A	2.023(3)	Ni1-O8	2.091(4)
Ni1-N2	2.119(4)	Ni1-N1	2.120(4)
Ni1-O1	2.119(3)	Ni1-O2	2.144(4)
O3A-Ni1-O8	93.65(14)	O3A-Ni1-N2	88.08(15)
O8-Ni1-N2	92.26(16)	O3A-Ni1-N1	88.72(16)
N2-Ni1-N1	176.76(17)	O3A-Ni1-O1	165.91(15)
O8-Ni1-O1	100.35(14)	N1-Ni1-O1	90.10(16)
Complex 2			
Ni1-O8	2.077(2)	Ni1-O7A	2.077(2)
Ni1-O1	2.086(2)	Ni1-N1	2.095(2)
Ni1-N2	2.112(2)	Ni1-N3	2.123(3)
O8-Ni1-O7A	93.32(9)	O8-Ni1-O1	90.86(9)
O7A-Ni1-O1	173.48(8)	O8-Ni1-N1	177.74(9)
O7A-Ni1-N1	88.82(9)	O1-Ni1-N1	86.95(9)
O8-Ni1-N2	89.38(9)	O7A-Ni1-N2	89.02(9)
O1-Ni1-N2	96.04(9)	N1-Ni1-N2	91.41(10)

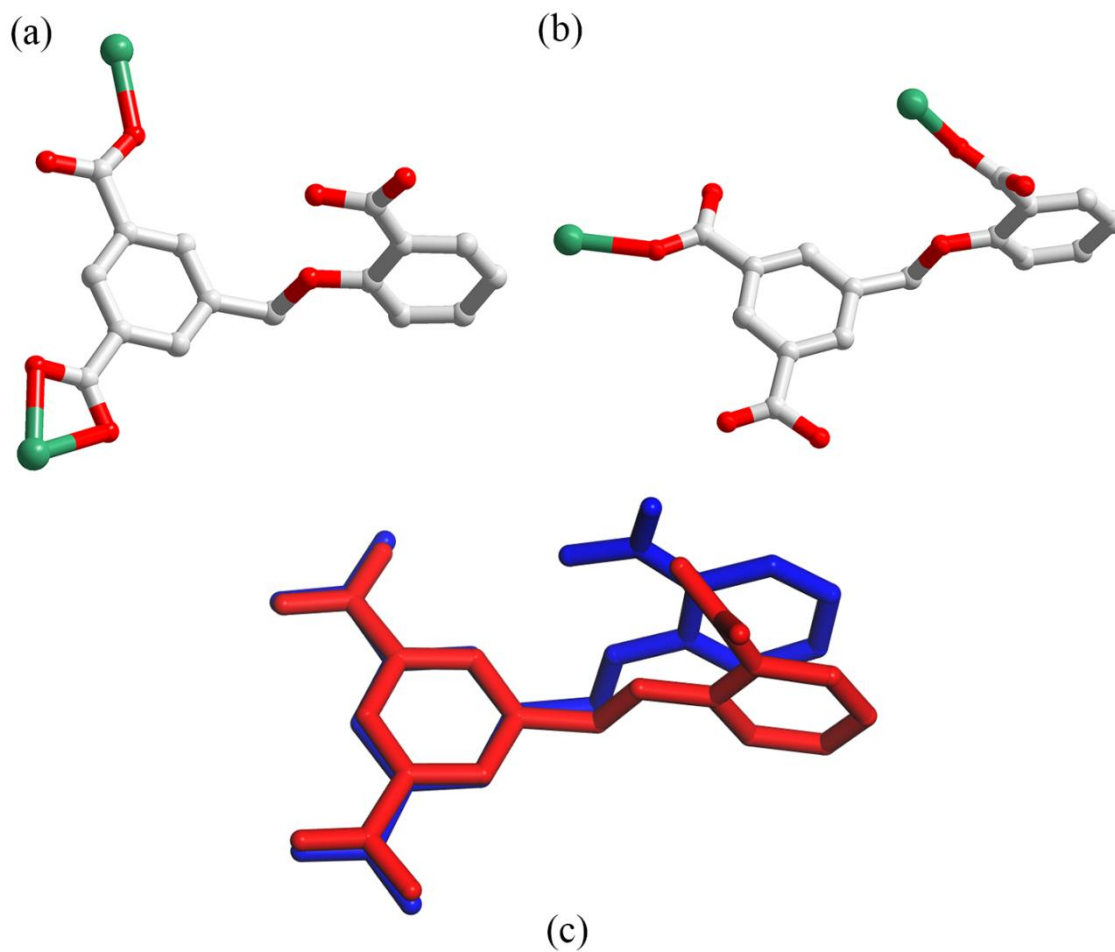


Figure S1 (a) and (b) The coordination modes of HL² ligands in the two complexes. (c) Overlay of L ligands in complex **1** (blue) and complex **2** (red).

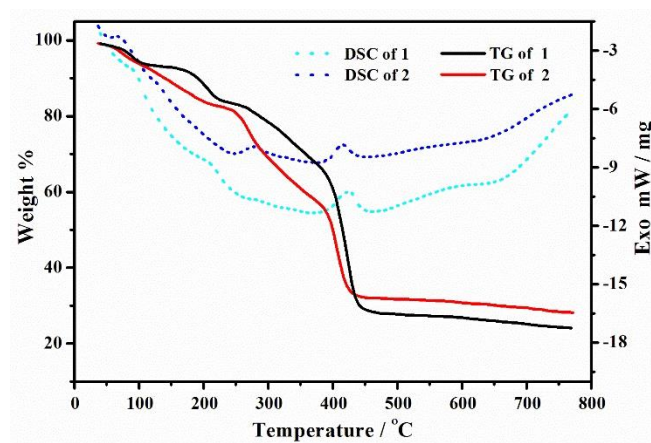


Figure S2 TG and DSC curves of two complexes.

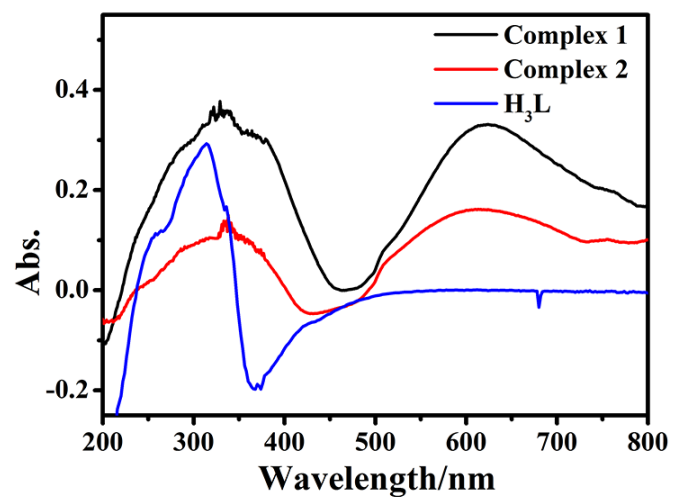


Figure S3. The solid-state UV-Vis spectra of H₃L and complexes at room temperature.