Chirality and absolute helicity in a pair of enantiomeric amino acid derivatives and their complexes: structures, chiroptical, and photoluminescent properties

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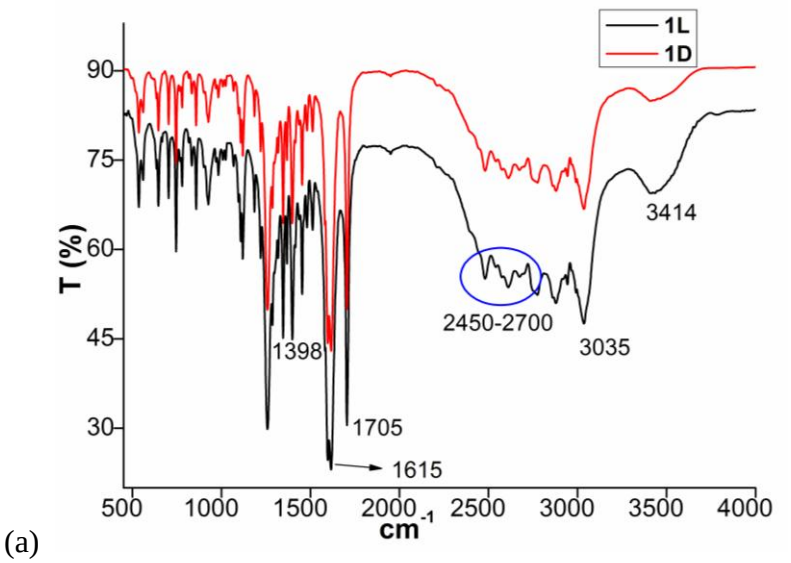
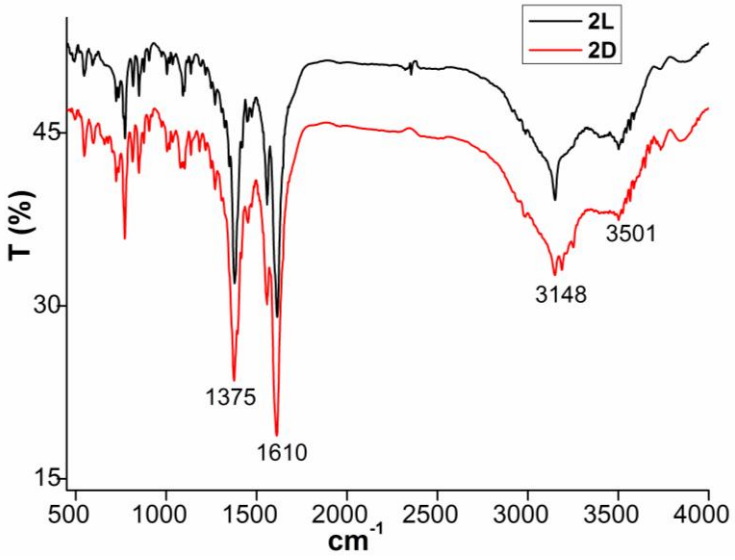


(a)



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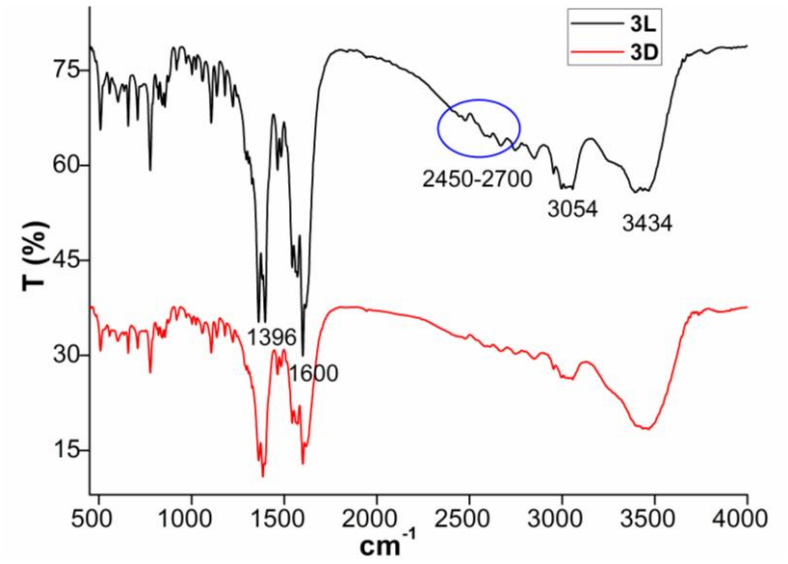


(c)

Figure S1. IR spectra of (a): **1L** and **1D**; (b): **2L** and **2D**; (c): **3L** and **3D**.

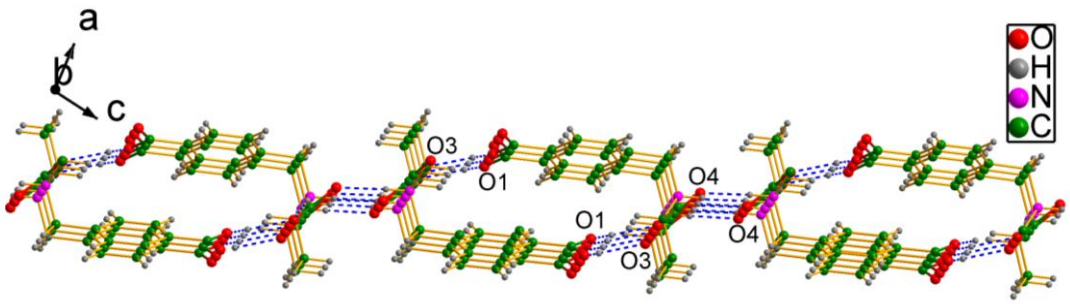


Figure S2. Perspective view of the 2D supramolecular structure of **1L** along *b*-axis.

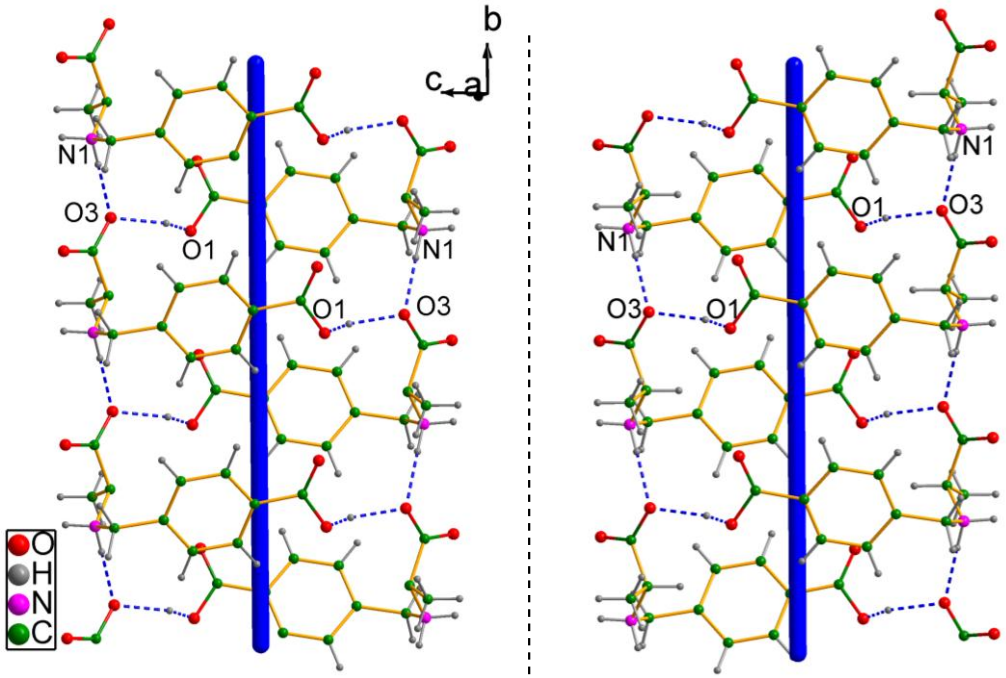


Figure S3. The absolute helicities of **1L** (left) and its enantiomer **1D** (right) on the direction of *b*-axis. The mirror is drawn as a dash line. **1L** is a single-stranded *P*-helix and **1D** is a single-stranded *M*-helix.

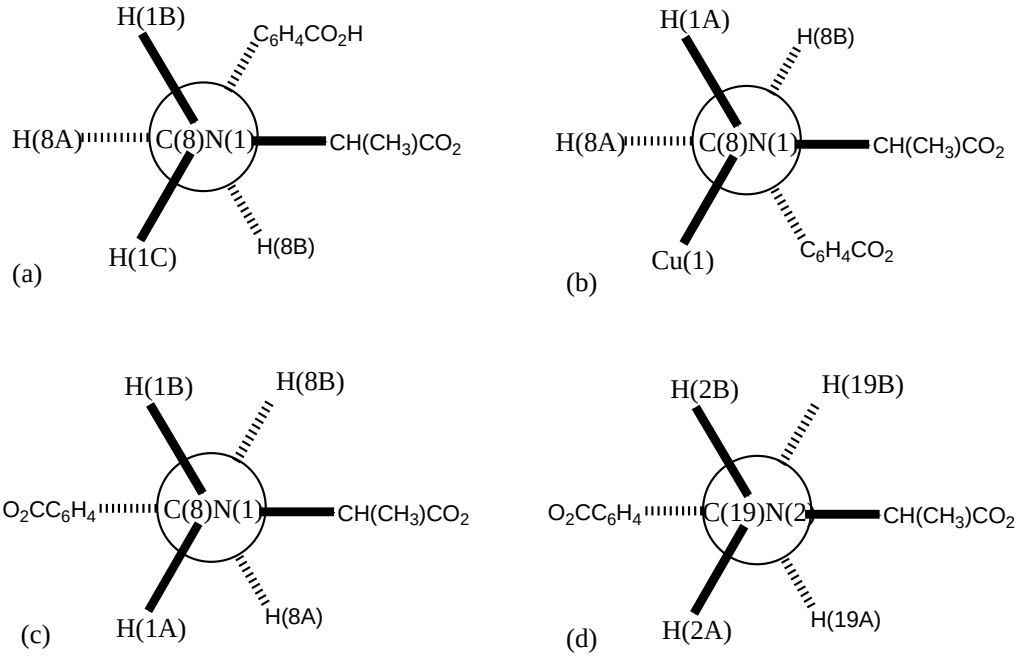


Figure S4. Newman projection models for (a): **1L**, gauche conformation; (b): **2L**, gauche conformation; (c) and (d): **3L**, staggered conformation.

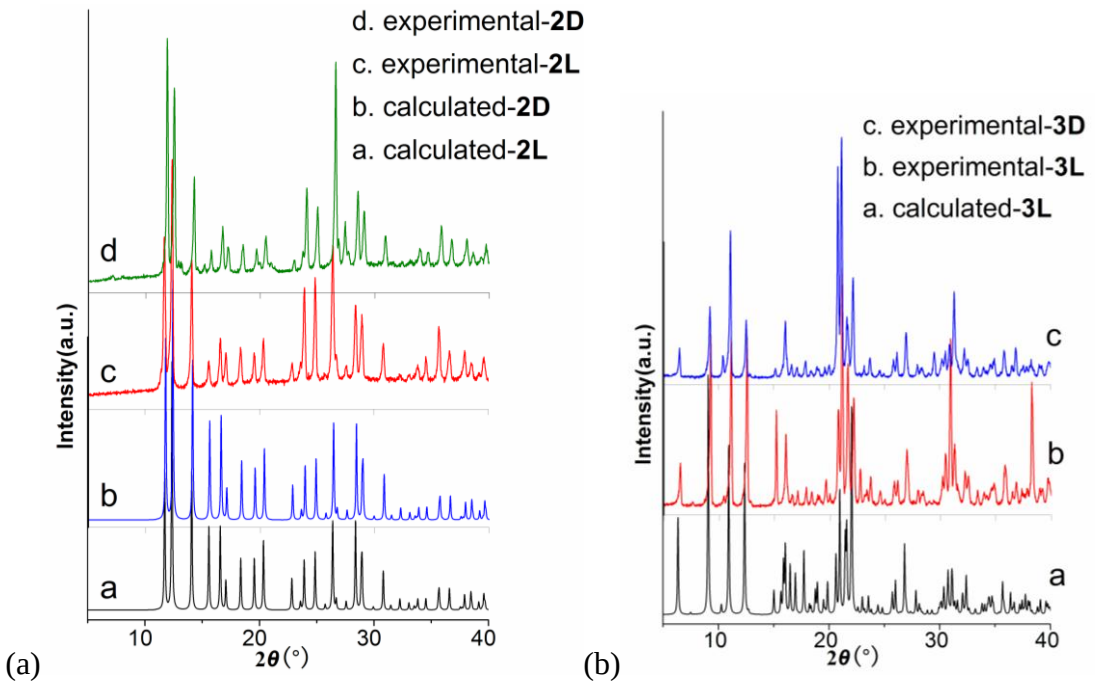


Figure S5. (a) Experimental and calculated powder XRD patterns of **2L** and **2D**. (b) Experimental and calculated powder XRD patterns of **3L** and **3D**.

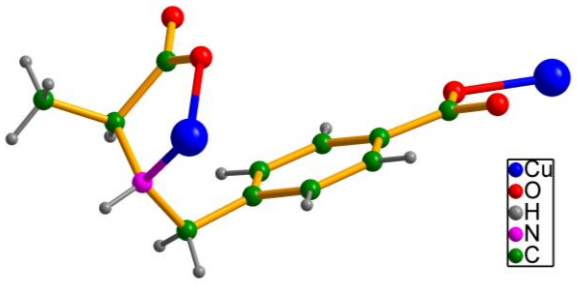


Figure S6. Coordination mode of cala^{2-} ligands exhibited in **2L** and **2D**.

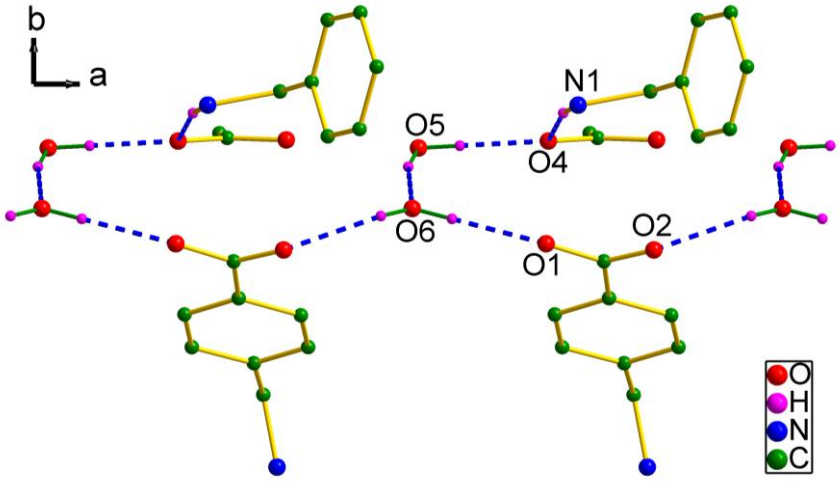


Figure S7. Hydrogen-bonding details in **2L**. The supramolecular structure is extended by intermolecular hydrogen bonds O(5)-H(5A)···O(4) (x,y-1,z), O(6)-H(6B)···O(1), O(6)-H(6C)···O(2) (x-1,y,z) along *a*-axis and by O(5)-H(5B)···O(6) (y,-x,z+1/4), $^{+}$N(1)-H(1A)···O(4) (-x+1,-y,z-1/2) along *b*-axis.

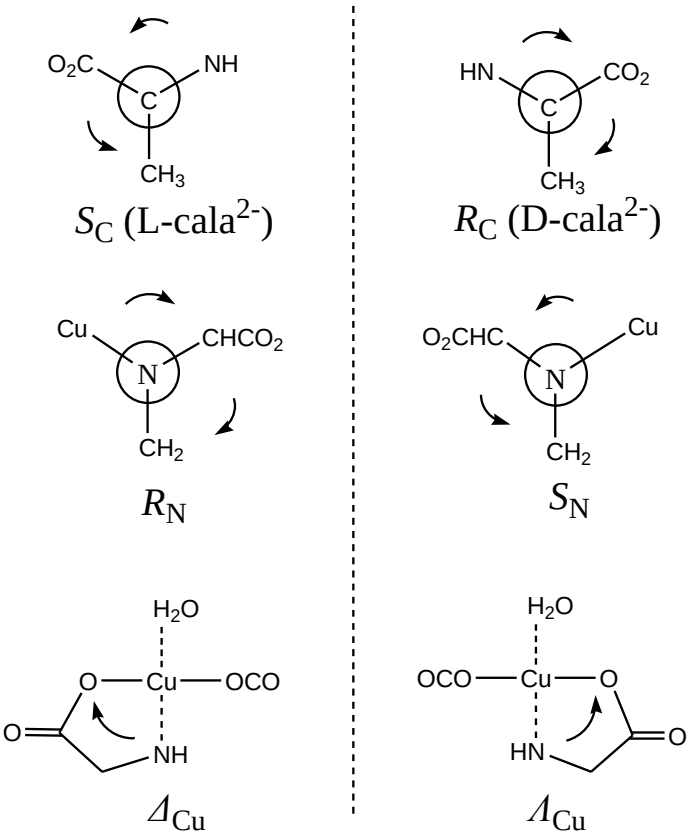


Figure S8. Absolute configurations of C(10), N(1) and Cu(1) in **2L** (left) and **2D** (right). The definition of the absolute configuration of Cu^{2+} is according to reference [S1]. Cu^{2+} adopts a distorted square coordination geometry. The dash line linking Cu^{2+} and donor atoms means the bond is pointing inward the paper plane. If the rotation from N to O (within the five-membered chelating ring) is clockwise, the absolute configuration of Cu^{2+} is defined as *Δ*. And so on, anticlockwise rotation is defined as *Λ*.

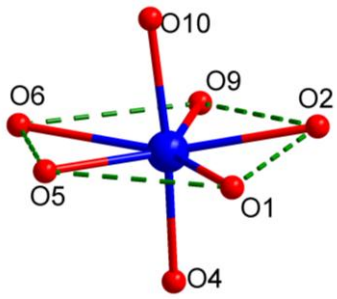


Figure S9. The coordination polyhedron of Cd^{2+} in **3L**.

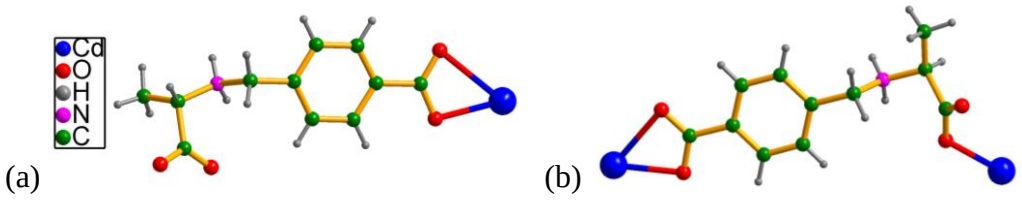


Figure S10. Coordination modes of two L-Hcala$^-$ ligands exhibited in **3L**.

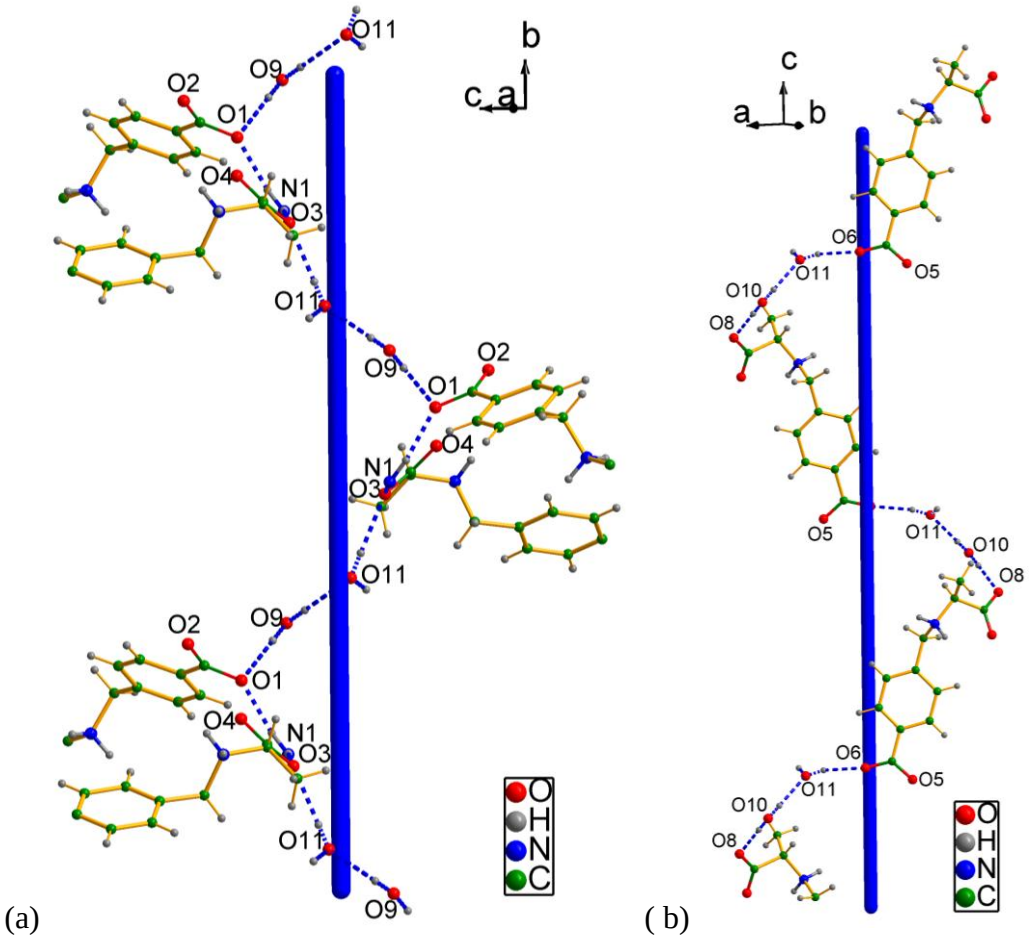


Figure S11. Hydrogen-bonding details in **3L**. (a) The bridging L-Hcala$^-$ ligand is extended by five hydrogen bonds O(9)-H(9A)···O(1) (x-1,y,z), O(9)-H(9B)···O(11) (-x+1,y-1/2,-z+3/2), O(11)-H(11D)···O(3) (x-3/2,-y+1/2,-z+2), N(1)-H(1A)···O(3) (x-1,y,z), N(1)-H(1B)···O(1) (x+1/2,-y+1/2,-z+2) in a head-and-tail manner along the direction of *b*-axis; (b) The terminal L-Hcala$^-$ ligand is extended by three hydrogen bonds O(10)-H(10B)···O(8) (-x+5/2,-y,z+1/2) , O(10)-H(10C)···O(11) (-x+2,y-1/2,-z+3/2), O(11)-H(11E)···O(6) (-x+1,y+1/2,-z+3/2) in a head-to-tail way along the direction of *c*-axis.

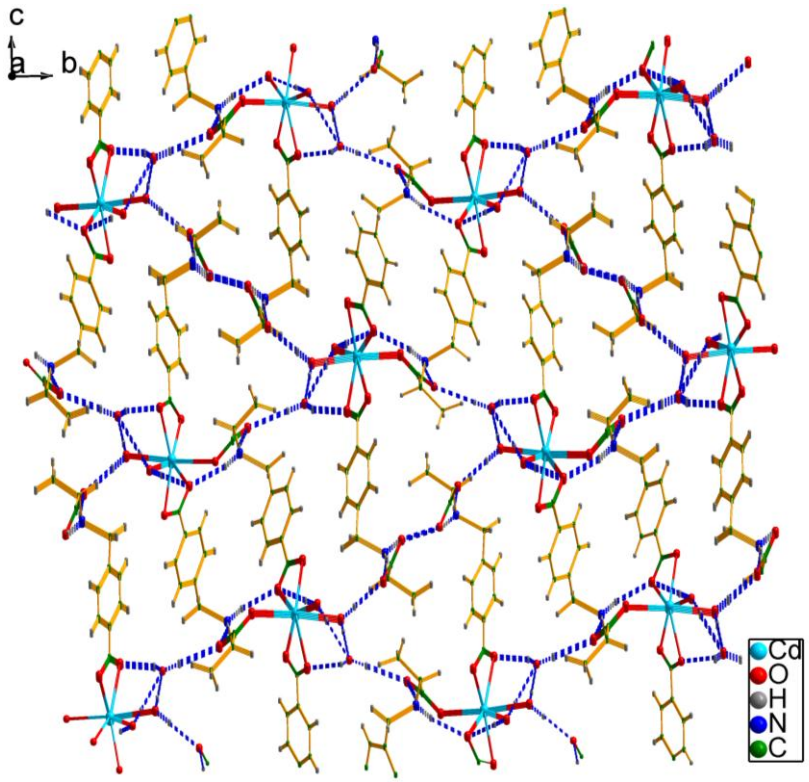
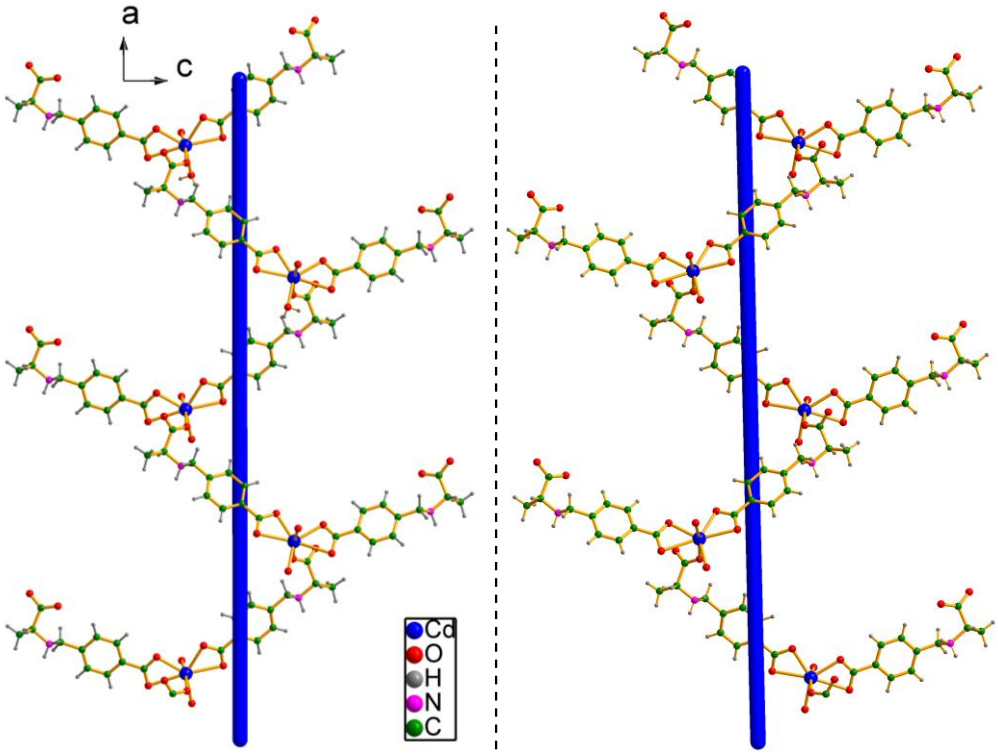


Figure S12. View of the 3D supramolecular structure of **3L** along *a*-axis.



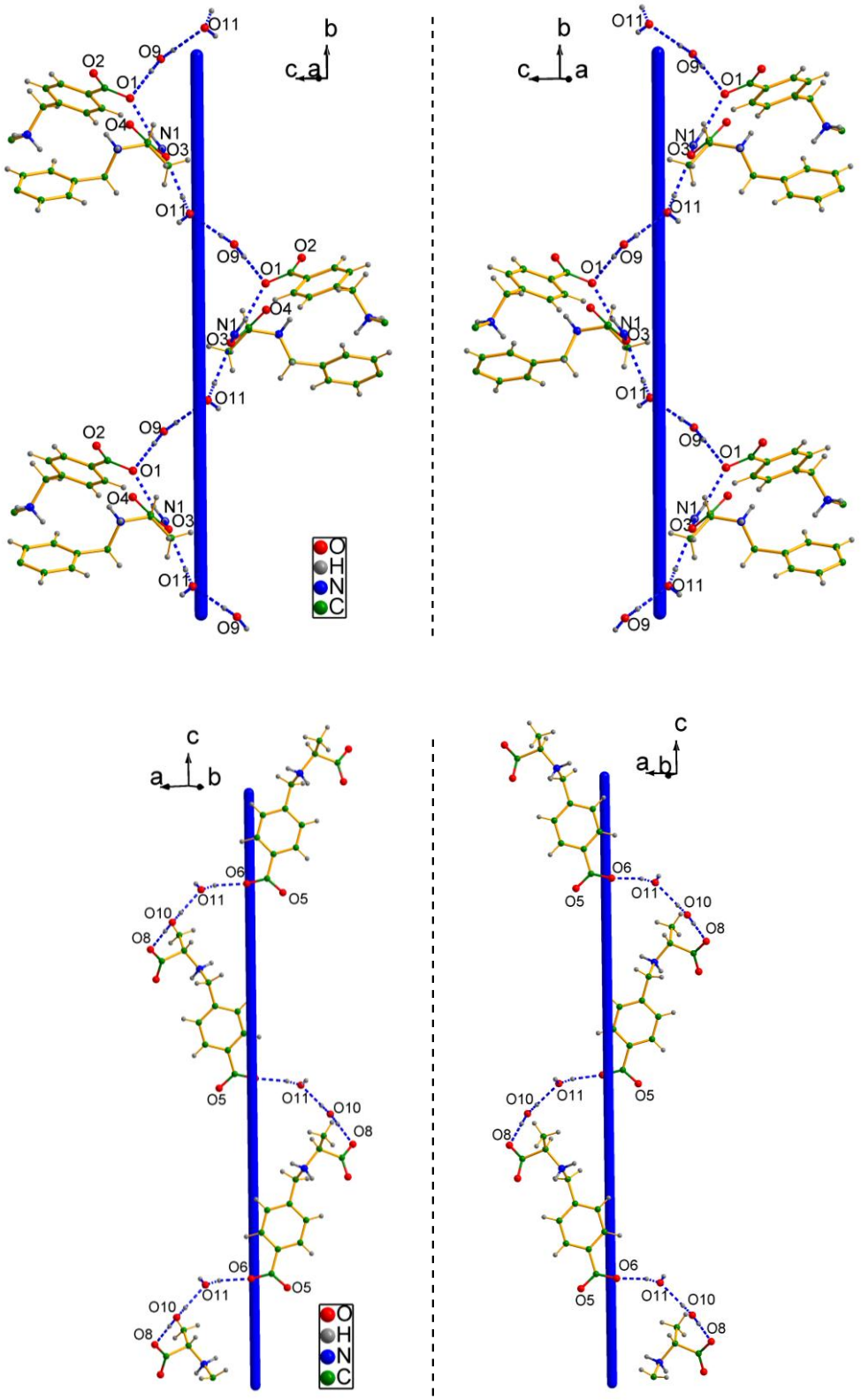


Figure S13. Comparison of the absolute helicities of **3L** (left) and its enantiomer **3D** (right) on the direction of *a*, *b* and *c*-axises, respectively. **3L** is M_a-M_b-P_c, while **3D** is P_a-P_b-M_c.

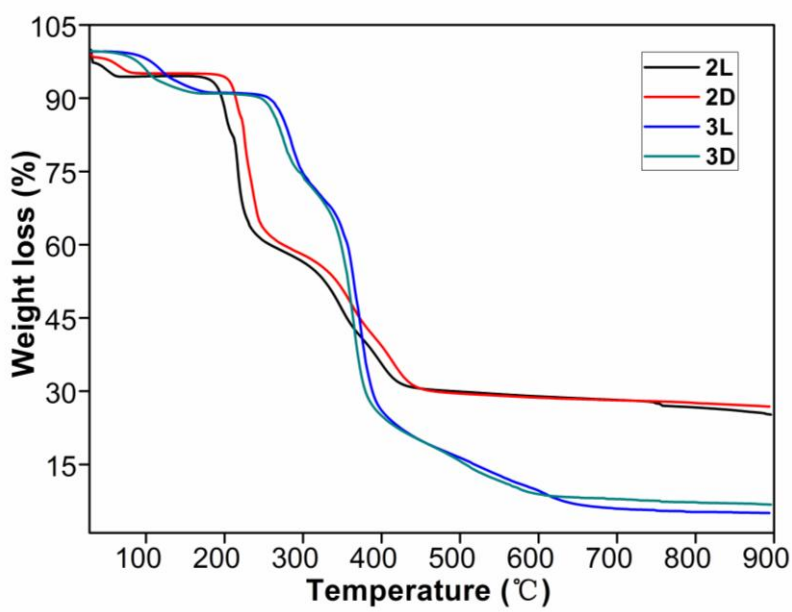


Figure S14. TGA curves of **2L**, **2D**, **3L** and **3D**.

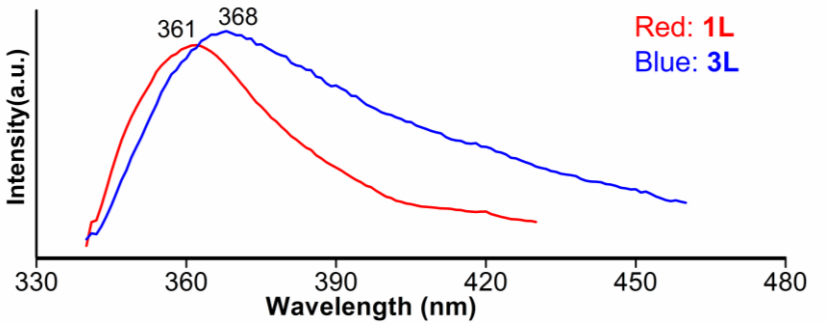


Figure S15. PL emission spectra of **1L** (λ_{ex} = 310nm) and **3L** (λ_{ex} = 320nm).

Table S1. Hydrogen-bonding parameters (Å and °) in **1L**, **2L**, **2D** and **3L**.

D-H···A	D-H	H···A	D···A	∠DHA
		1L		
O(1)-H(1A)...O(3)#1	0.82	1.78	2.593(2)	168.6
N(1)-H(1B)...O(3)#2	0.90	1.86	2.759(3)	179.0
N(1)-H(1C)...O(4)#3	0.90	1.92	2.783(3)	161.4
		2L		
O(5)-H(5A)...O(4)#3	0.85	1.82	2.668(4)	179.7

O(5)-H(5B)...O(6)#4	0.85	1.88	2.703(5)	163.3
O(6)-H(6C)...O(2)#5	0.85	2.11	2.871(4)	148.0
O(6)-H(6B)...O(1)	0.85	2.02	2.867(4)	179.6
N(1)-H(1A)...O(4)#6	0.91	2.15	3.048(4)	168.0
		2D		
O(5)-H(5A)...O(4)#3	0.85	1.82	2.668(4)	179.4
O(5)-H(5B)...O(6)	0.85	1.94	2.698(5)	147.7
O(6)-H(6B)...O(1)#4	0.85	2.02	2.868(4)	179.6
O(6)-H(6C)...O(2)#5	0.85	2.04	2.881(4)	167.6
N(1)-H(1A)...O(4)#6	0.91	2.16	3.051(4)	167.7
		3L		
O(9)-H(9A)...O(1)#3	0.85	1.96	2.811(6)	179.6
O(9)-H(9B)...O(11)#4	0.85	2.15	2.997(6)	178.9
O(10)-H(10B)...O(8)#5	0.85	1.80	2.655(6)	179.5
O(10)-H(10C)...O(11)#6	0.85	2.00	2.850(6)	179.8
O(11)-H(11D)...O(3)#1	0.85	2.02	2.870(6)	179.3
O(11)-H(11E)...O(6)#7	0.85	2.04	2.831(7)	153.7
N(1)-H(1A)...O(3)#3	0.90	1.94	2.818(5)	165.6
N(1)-H(1B)...O(1)#8	0.90	1.92	2.786(6)	159.7
N(2)-H(2A)...O(7)#9	0.90	2.01	2.808(6)	146.5
N(2)-H(2B)...O(8)#3	0.90	1.93	2.808(6)	166.1

Symmetry codes: for **1L** #1 -x+1,y-1/2,-z+2. #2 x,y-1,z. #3 -x,y-1/2,-z+1. **2L** #3 x,y-1,z. #4 y,-x,z+1/4. #5 x-1,y,z. #6 -x+1,-y,z-1/2. **2D** #3 x+1,y,z. #4 -y+2,x,z+1/4. #5 -y+1,x,z+1/4. #6 y,-x+1,z-1/4. **3L** #1 x-3/2,-y+1/2,-z+2. #3 x-1,y,z. #4 -x+1,y-1/2,-z+3/2. #5 -x+5/2,-y,z+1/2. #6 -x+2,y-1/2,-z+3/2. #7 -x+1,y+1/2,-z+3/2. #8 x+1/2,-y+1/2,-z+2. #9 x-1/2,-y+1/2,-z+1.

[S1] Zhang, H. *Coordination Chemistry—Principles and Applications*; Chemical Industry Press, Beijing, 2010.