Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Supporting Information

Vapor-induced Chiroptical Switching in Chiral Cyclometalated Platinum(II) Complexes with Pinene Functionalized C^N^N Ligands

Xiao-Peng Zhang, Tao Wu, Jian Liu, Jing-Xuan Zhang, Cheng-Hui Li*, Xiao-Zeng You*

†State Key laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing National Laboratory of Microstructures Nanjing University, Nanjing 210093, People's Republic of China. E-mail:chli@nju.edu.cn (C. –H. Li); youxz@nju.edu.cn (X.-Z. You.)

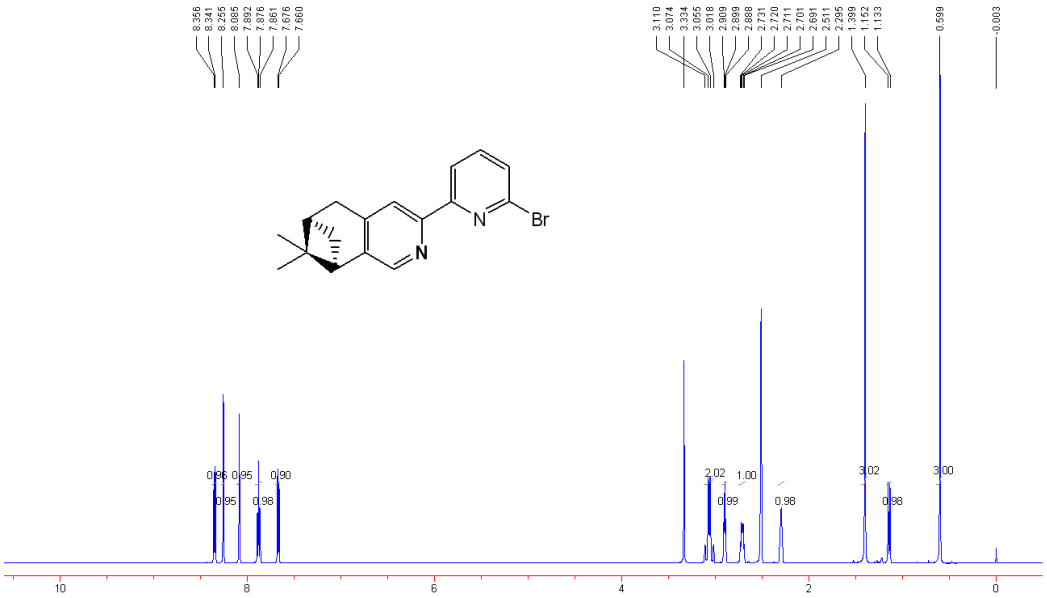

Fig. S1 ^{1}H NMR spectrum of (-)-4,5-pinene-6'-bromo-2,2'-bipyridine.

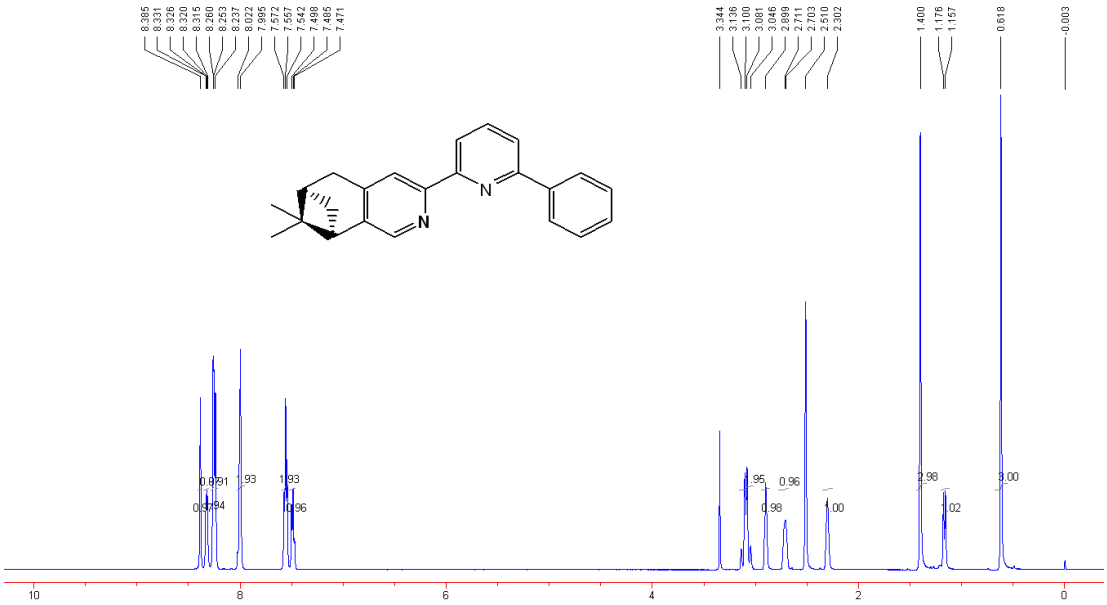

Fig. S2 ^{1}H NMR spectrum of (-)-4,5-pinene-6'-phenyl-2,2'-bipyridine (L_a).

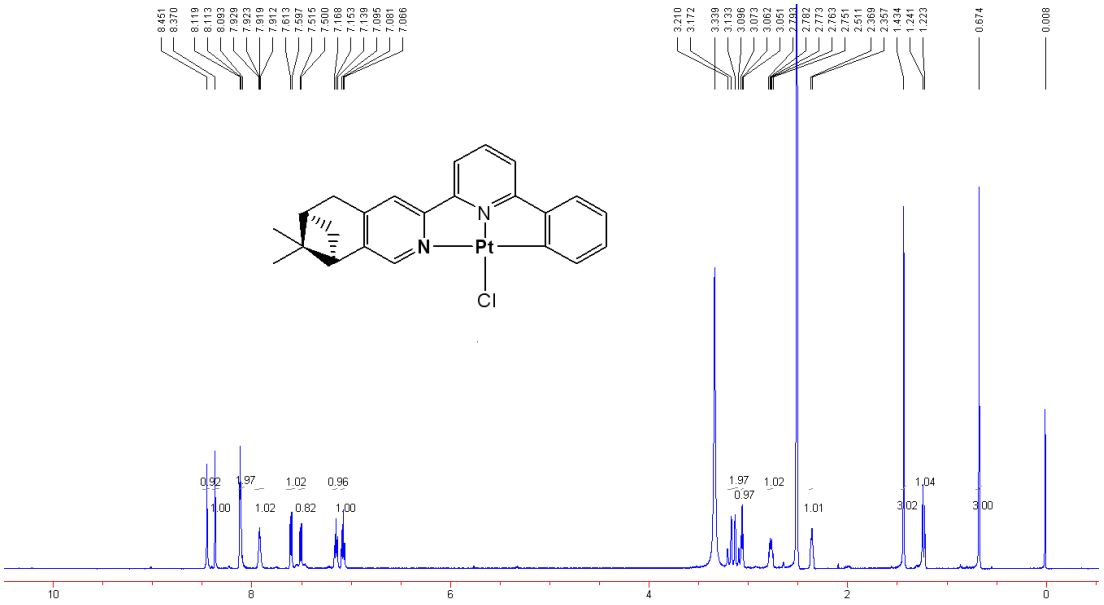

Fig. S3 ^{1}H NMR spectrum of Pt(L_a)Cl.

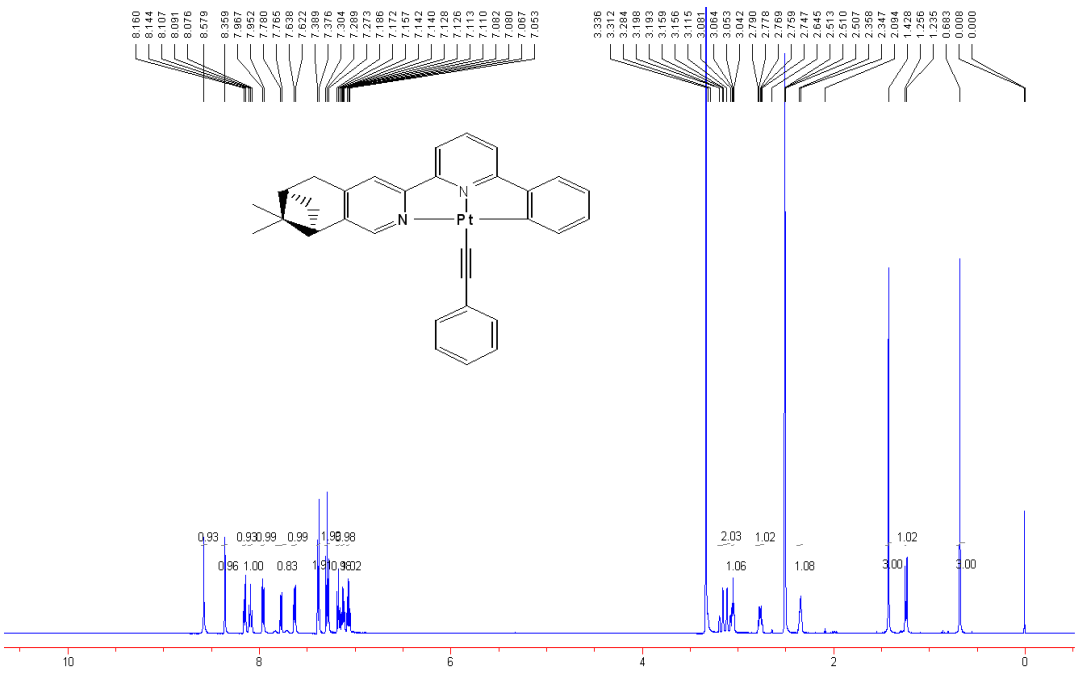

Fig. S4 ^{1}H NMR spectrum of Pt(L_a)(C≡C-Ph) (**1a**).

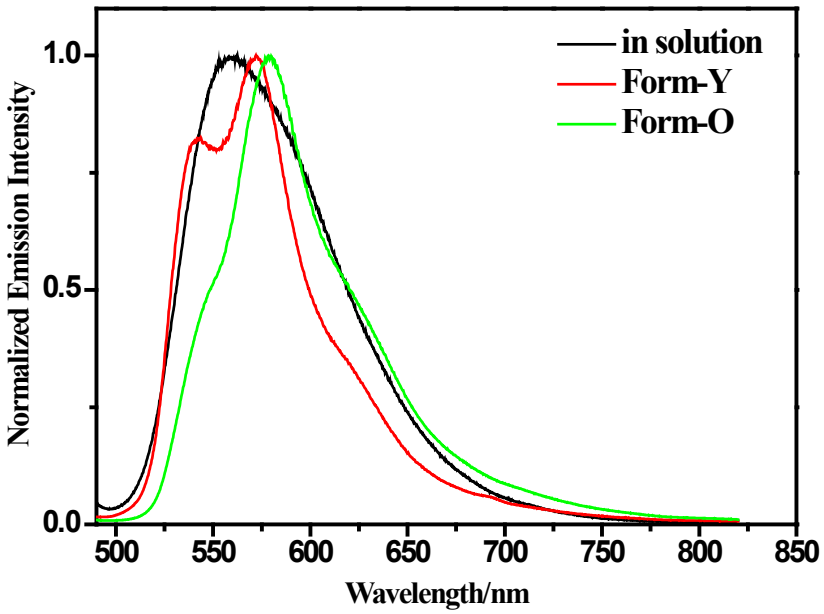

Fig. S5 Emission spectra of **1a** in solution (10^{-5} mol·L^{-1}) and different solid-state forms at 298K (in acetonitrile solution at 298K, λ_{ex} =420nm; **Form-Y**: yellow crystallites, λ_{ex} = 460 nm; **Form-O**: orange crystallites, λ_{ex} = 470 nm).

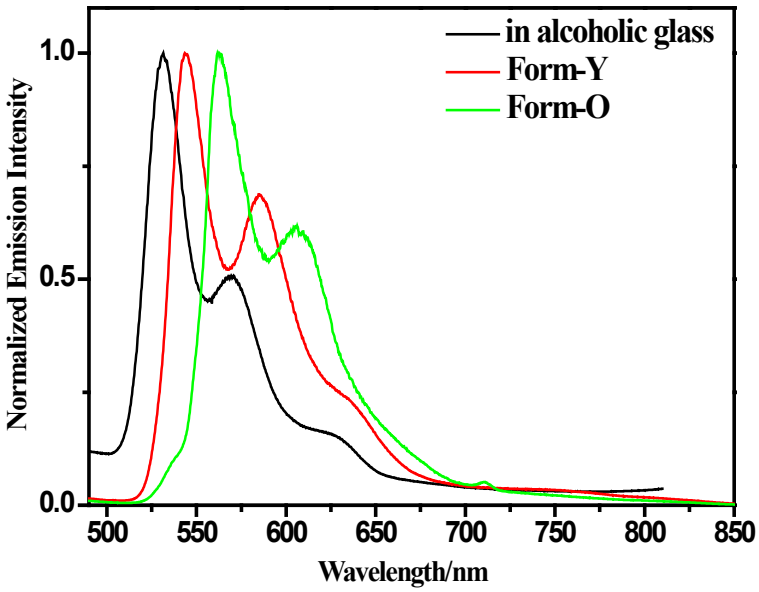

Fig. S6 Emission spectra of **1a** in alcoholic glass (10^{-5} mol·L^{-1}) and different solid-state forms at 77K (in MeOH : EtOH (v/v = 1:4) glass, λ_{ex} =420nm; **Form-Y**: yellow crystallites, λ_{ex} = 460 nm; **Form-O**: orange crystallites, λ_{ex} = 470 nm).

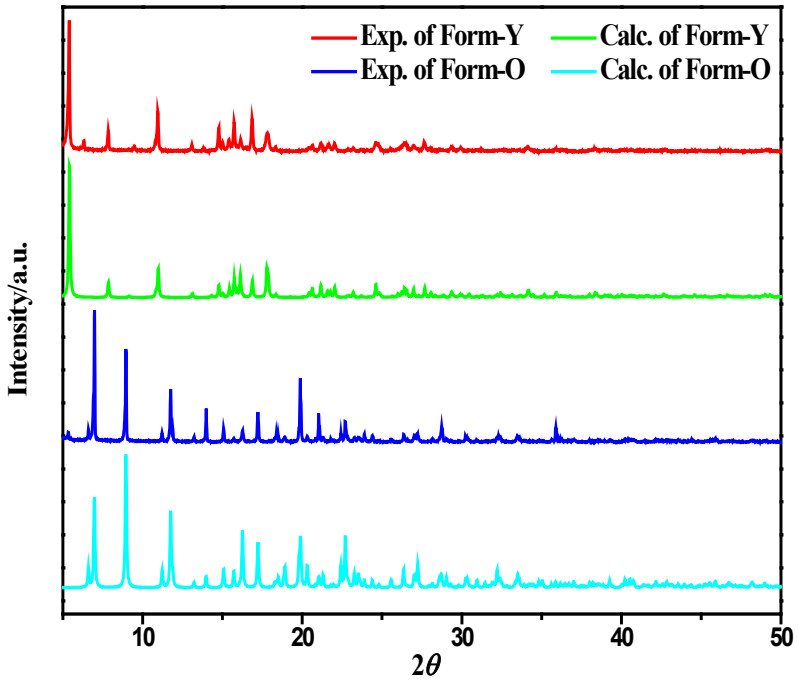

Fig. S7 Simulated and experimental XRD patterns of complex **1a** with different forms. (**Form-Y**: yellow crystallites; **Form-O**: orange crystallites)

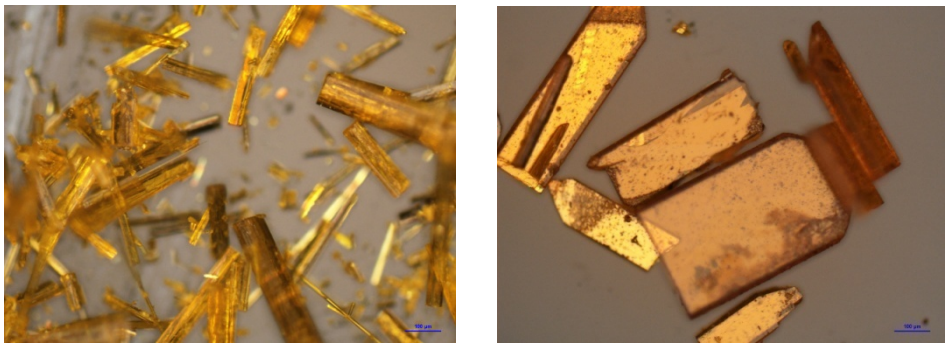

Fig. S8 Crystal pictures of **1a-From-Y** (left) and **1a-Form-O** (right).

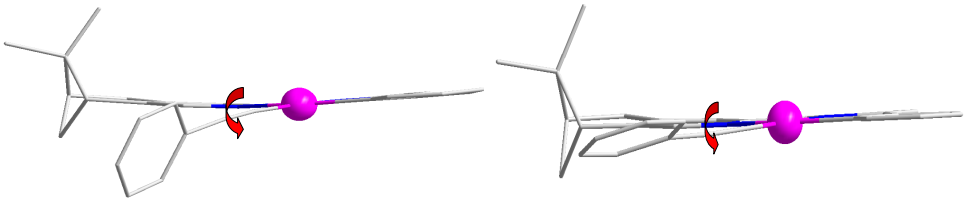

Fig. S9 Absolute configurations of **1a-Form-Y** (left) and **1a-Form-O** (right) based on skew-line system, and both of them are Λ.

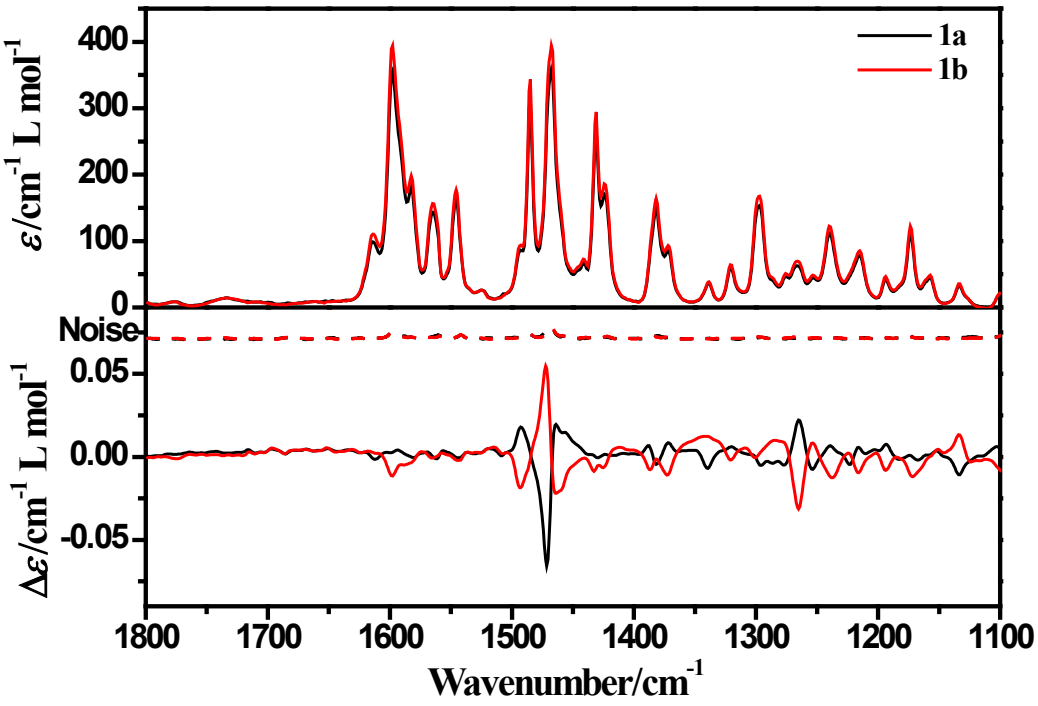

Fig. S10 IR and VCD spectra of complexes **1a** and **1b** in $CDCl_3$ solution.

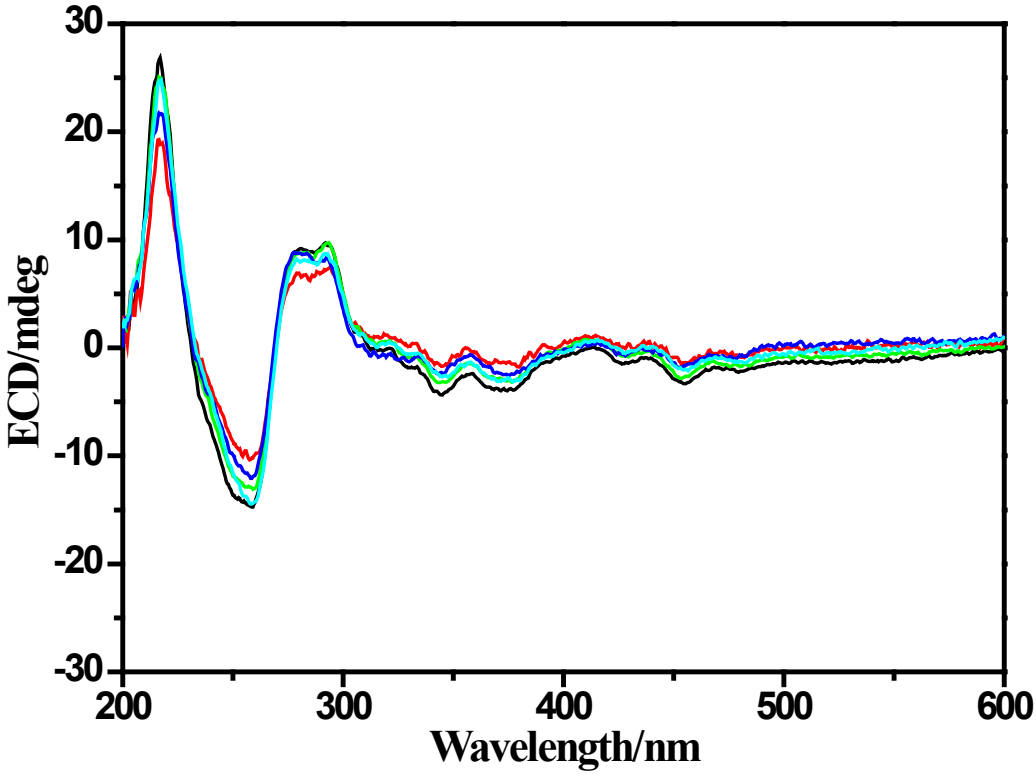

Fig. S11 Five groups solid-state ECD spectra of **Form-Y** of **1a** under the same measuring condition.

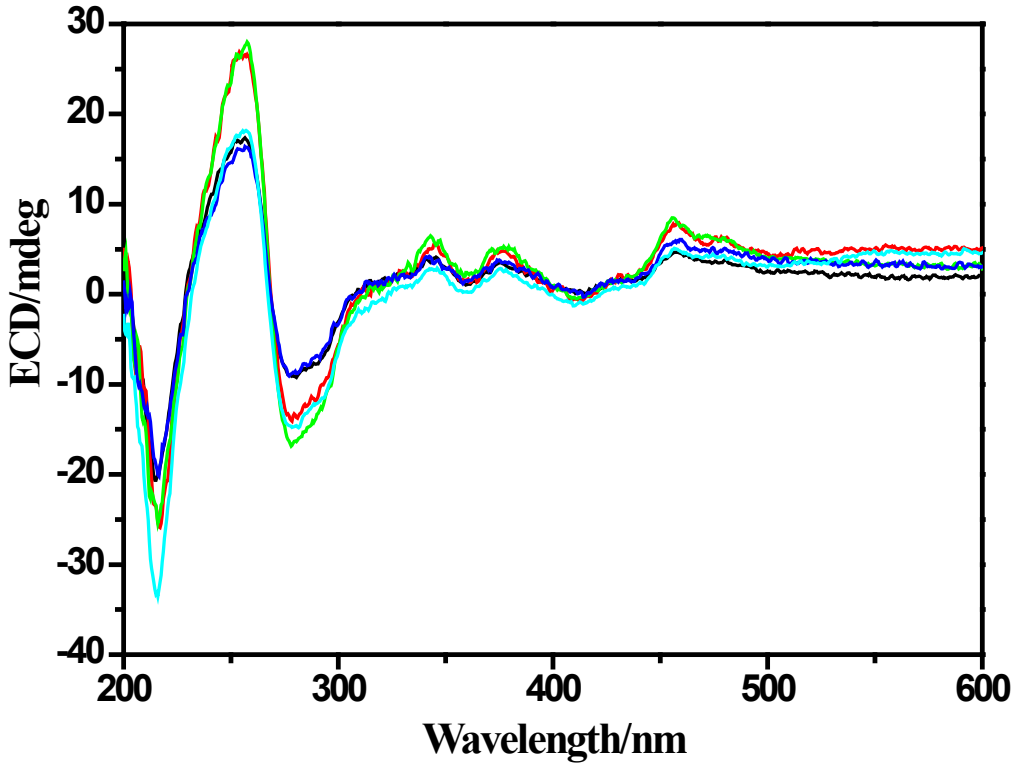

Fig. S12 Five groups solid-state ECD spectra of **Form-Y** of **1b** under the same measuring condition.

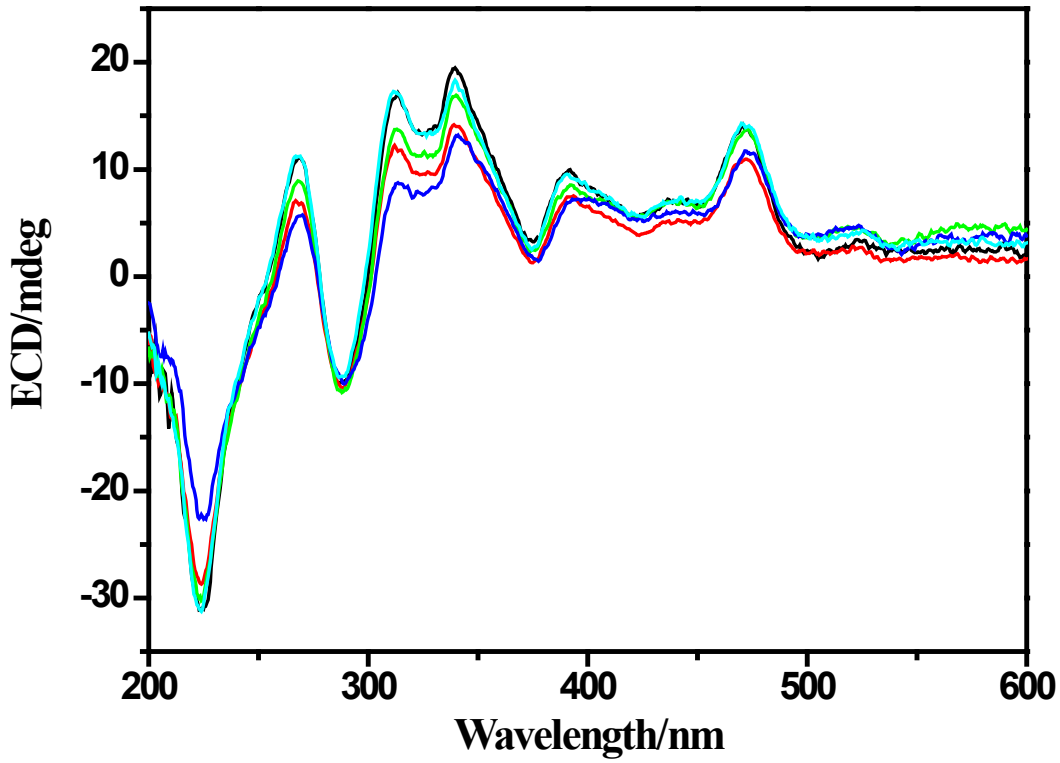

Fig. S13 Five groups solid-state ECD spectra of **Form-O** of **1a** under the same measuring condition.

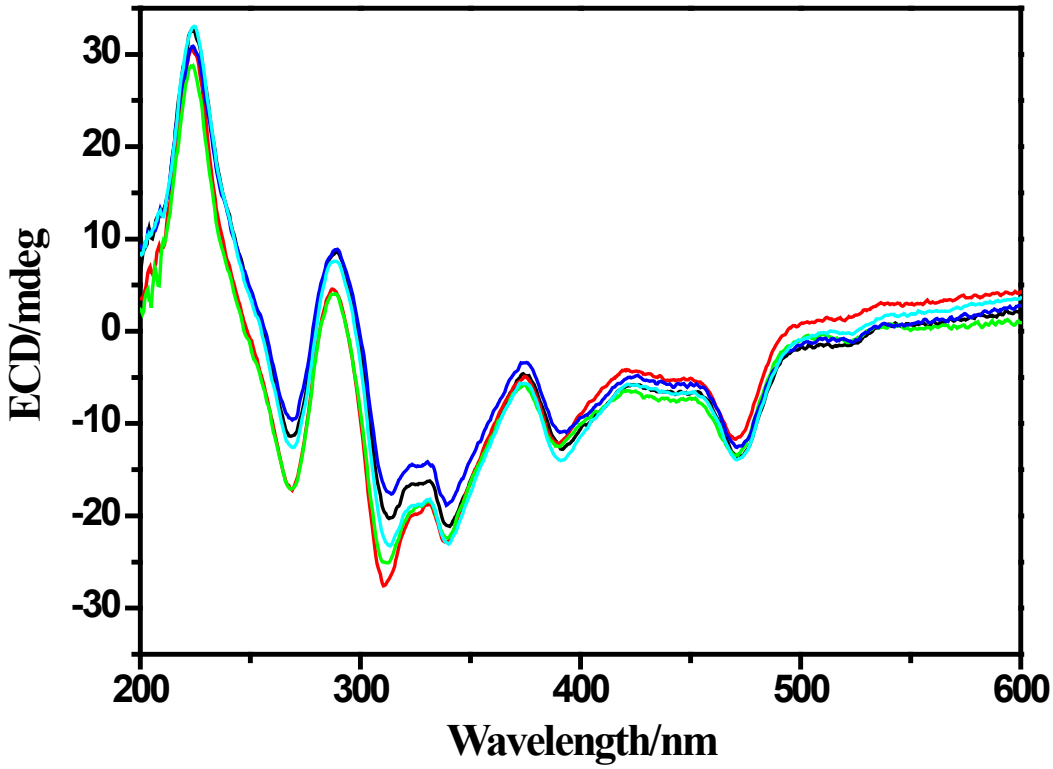

Fig. S14 Five groups solid-state ECD spectra of **Form-O** of **1b** under the same measuring condition.

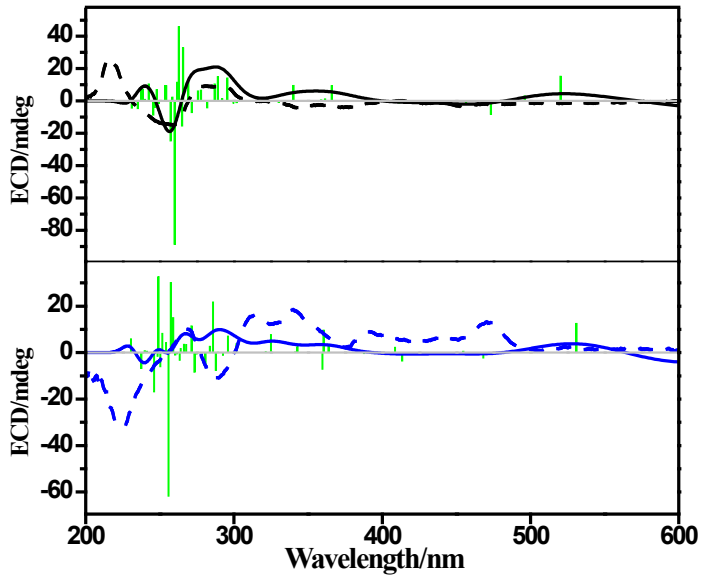

Fig. S15 Computed ECD spectra (solid line) of **Form-Y** (black) and **Form-O** (blue) of complex **1a** compared to observed solid-state ECD spectra (dash line). The green column is the computed rotatory strength.

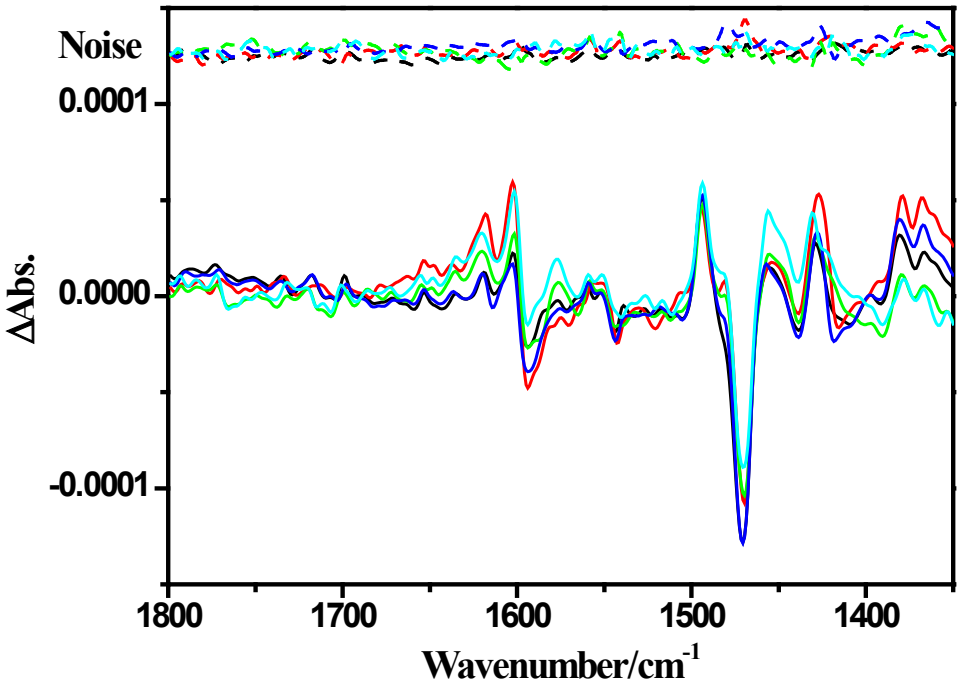

Fig. S16 Five groups solid-state VCD spectra of **Form-Y** of **1a** under the same measuring condition (solid line: VCD spectra; dashed line: noise level).

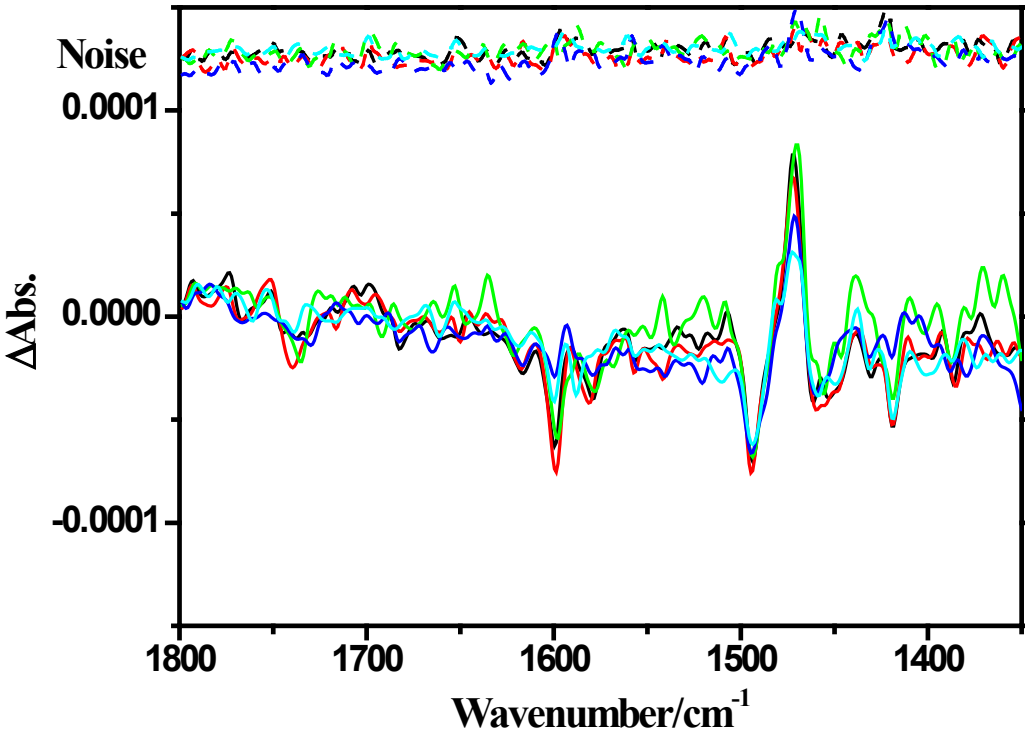

Fig. S17 Five groups solid-state VCD spectra of **Form-Y** of **1b** under the same measuring condition (solid line: VCD spectra; dashed line: noise level).

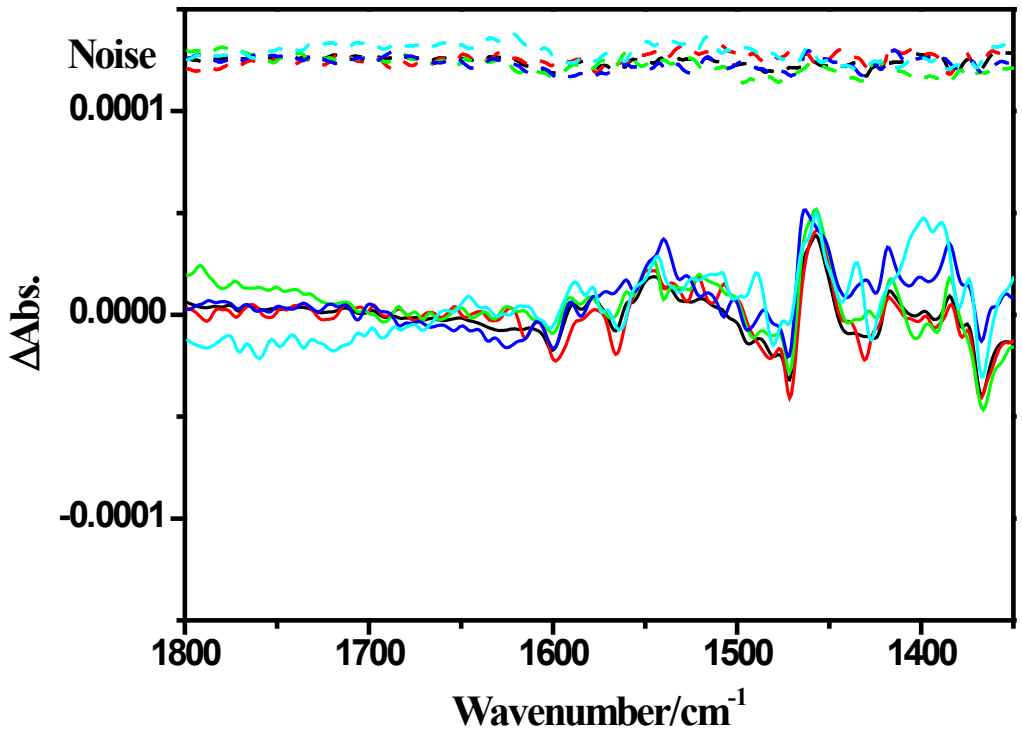

Fig. S18 Five groups solid-state VCD spectra of **Form-O** of **1a** under the same measuring condition (solid line: VCD spectra; dashed line: noise level).

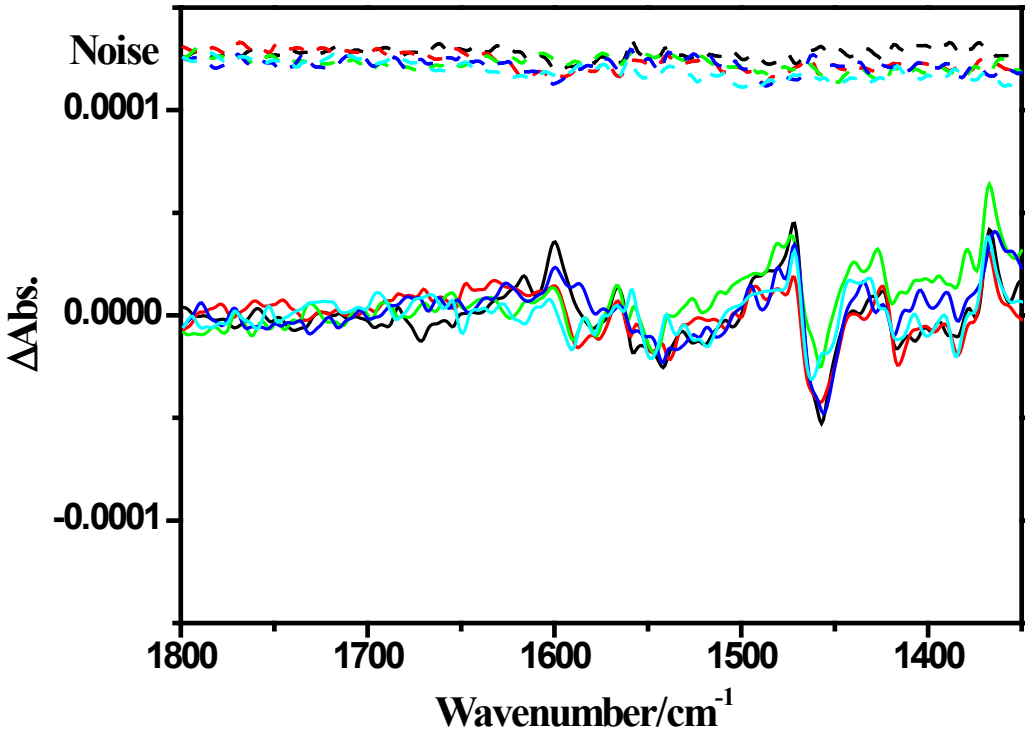

Fig. S19 Five groups solid-state VCD spectra of **Form-O** of **1b** under the same measuring condition (solid line: VCD spectra; dashed line: noise level).

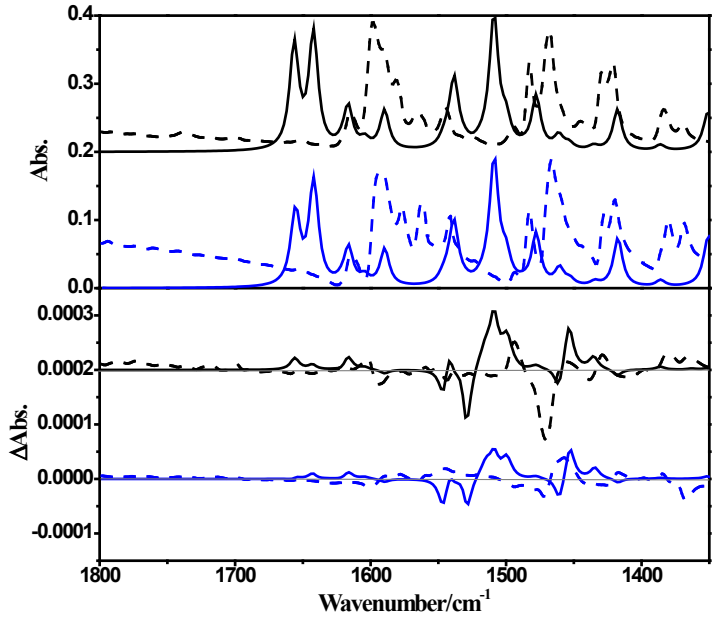

Fig. S20 Computed IR and VCD spectra (solid line) of **Form-Y** (black) and **Form-O** (blue) of complex **1a** compared to observed solid-state VCD spectra (dash line).

Table S1 Structural parameters both solid-state forms of complexes **1a** and **1b** determined by X-ray single crystal diffraction.

Bond Length	**1a-Form-Y**	**1a-Form-O**	**1b-Form-Y**	**1b-Form-O**
Pt1−C1	1.986(5)	1.991(4)	2.007(6)	1.993(10)
Pt1−C2	1.957(5)	1.975(4)	1.985(12)	1.965(10)
Pt1−N1	1.988(4)	1.988(3)	1.968(10)	1.968(8)
Pt1−N2	2.111(4)	2.103(3)	2.088(10)	2.086(9)
Bond Angles	**1a-Form-Y**	**1a-Form-O**	**1b-Form-Y**	**1b-Form-O**
C1−Pt1−C2	99.6(2)	98.95(17)	100.2(4)	100.1(5)
C1−Pt1−N1	82.44(18)	82.31(15)	81.3(3)	81.1(4)
C1−Pt1−N2	160.75(16)	160.88(15)	158.8(4)	159.5(4)
C2−Pt1−N1	176.7(2)	178.23(15)	177.9(4)	178.3(4)
C2−Pt1−N2	99.68(19)	100.16(13)	101.0(5)	100.4(4)
N1−Pt1−N2	78.35(16)	78.57(11)	77.4(4)	78.5(3)