Supporting Information

Mechano-induced Luminescent and Chiroptical Switching in Chiral Cyclometalated Platinum(II) Complexes

Xiao-Peng Zhang, Jin-Feng Mei, Jian-Cheng Lai, Cheng-Hui Li,* Xiao-Zeng You*

†State Key laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Collaborative Innovation Center of Advanced 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.)

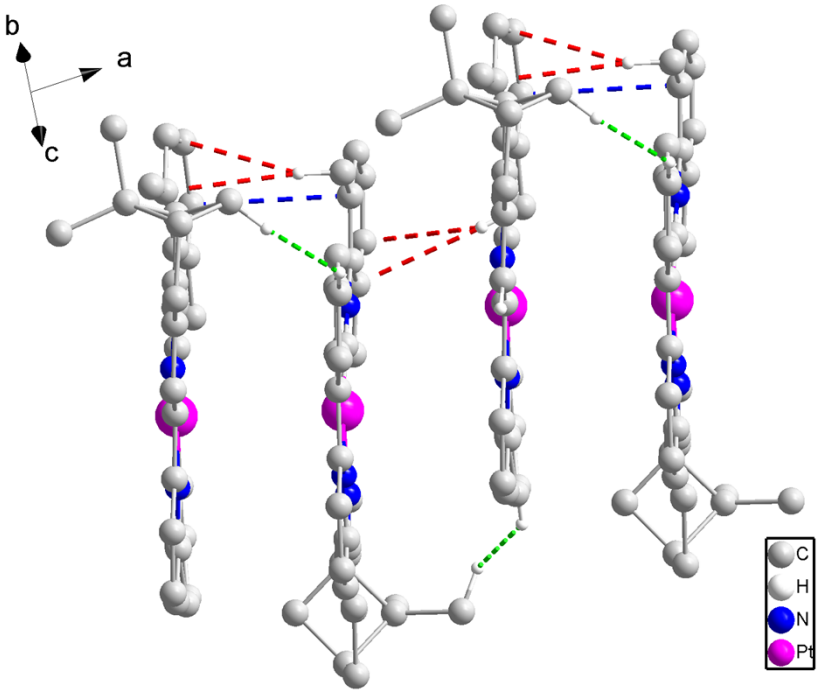

Fig. S1 The packing diagram of (−)-**1-Form-Y** along *a*-axis with blue dashed lines indicating the π–π interaction, red dashed lines indicating the C−H···π interaction and green dashed lines indicating the C−H···H−C interaction. The H-atoms not involved in C−H···π and C−H···H−C interactions are omitted for clarity.

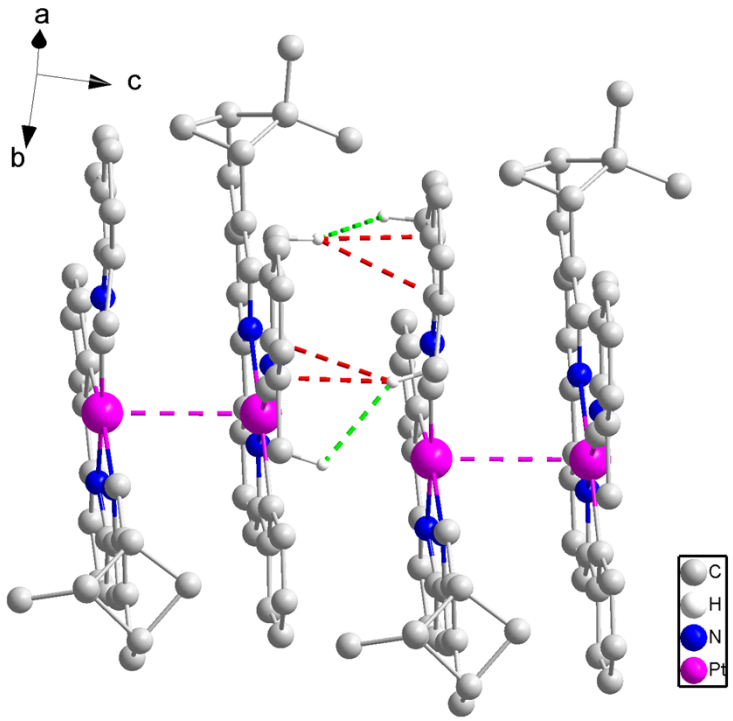

Fig. S2 The packing diagram of (−)-**1-Form-R** along *c*-axis with red dashed lines indicating the C−H···π interaction, magenta dashed lines indicating the Pt···Pt interaction and green dashed lines indicating the C−H···H−C interaction. The H-atoms not involved in C−H···π and C−H···H−C interactions are omitted for clarity.

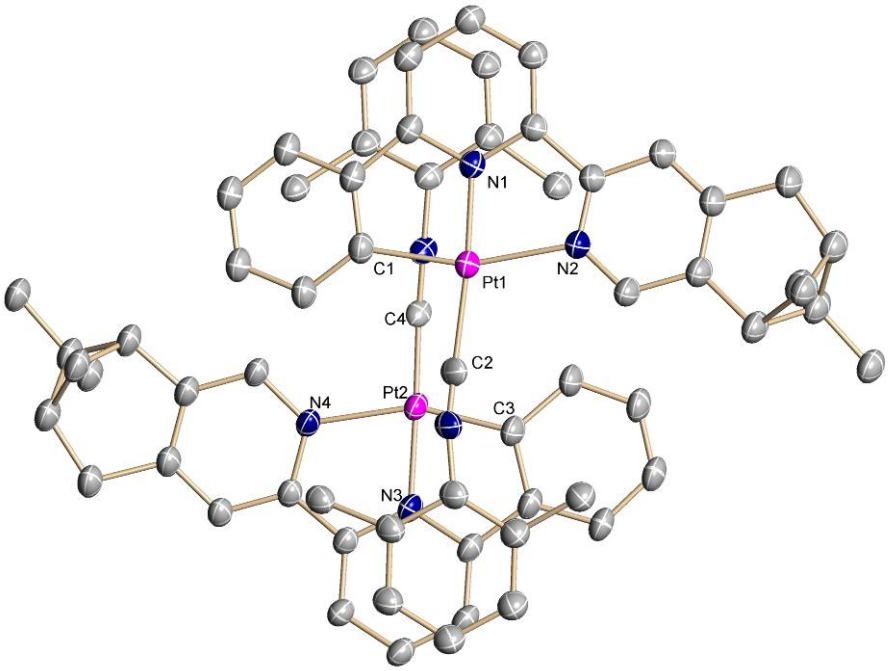

Fig. S3 ORTEP plot of (−)-**2**. The thermal ellipsoids are drawn at 30% probability (Hydrogen atoms, solvent molecules and anions are omitted for clarity).

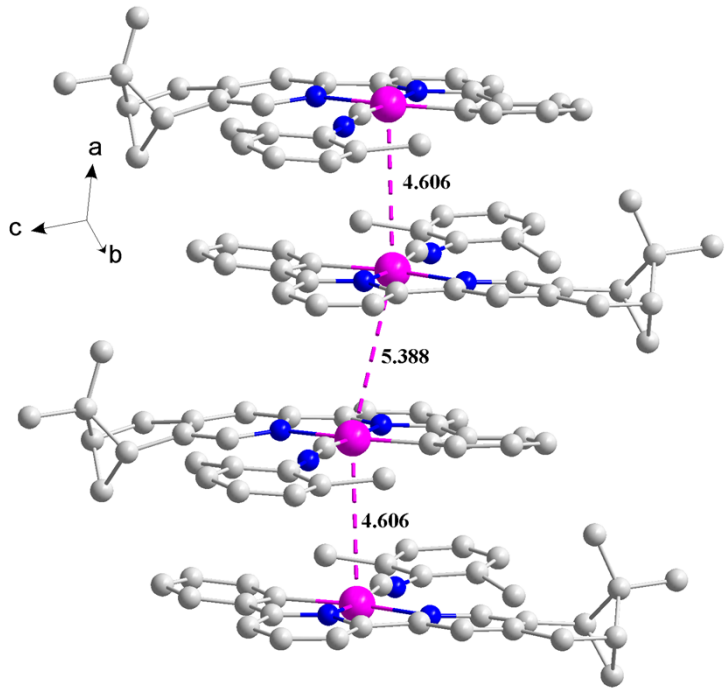

Fig. S4 Crystal packing diagram of (−)-**2** depicting the Pt···Pt distances.

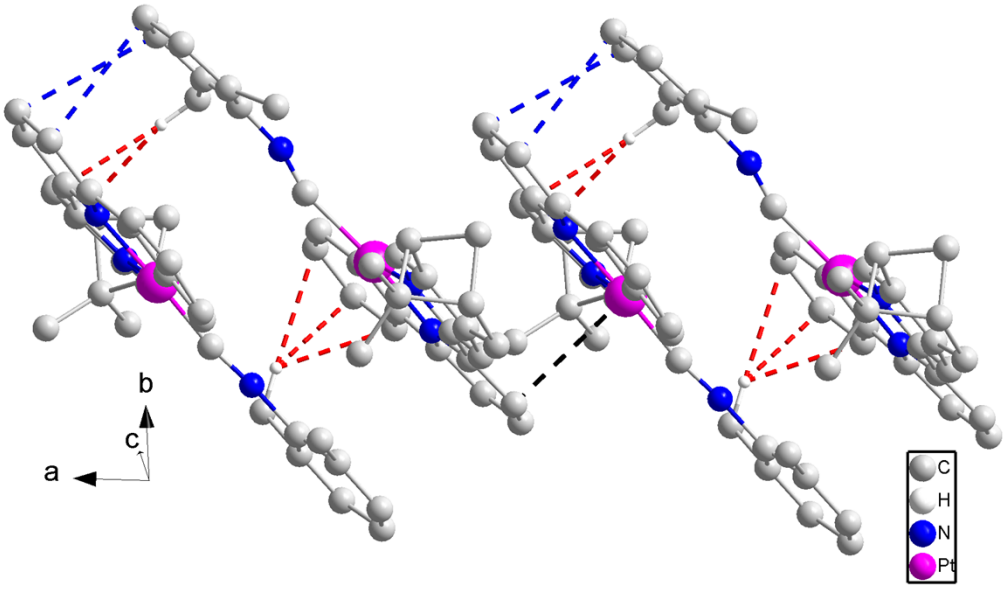

Fig. S5 The packing diagram of (−)-**2** along *a*-axis with blue dashed lines indicating the π–π interaction, black dashed lines indicating the Pt–π interaction and red dashed lines indicating the C–H···π interaction. The H-atoms not involved in C–H···π and C–H···H–C interactions are omitted for clarity.

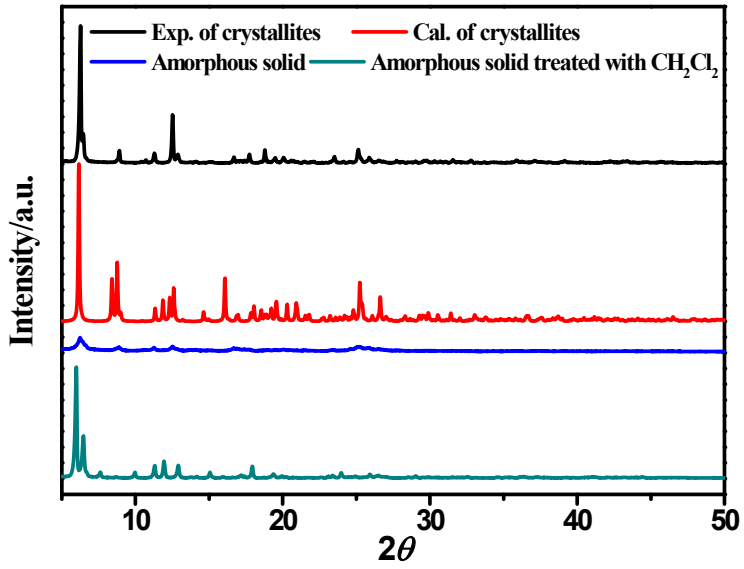

Fig. S6 Simulated and experimental XRD patterns of (−)-**2** as well as in the reversible mechanochromic process (Amorphous solid: crystallites after grinding for tens of seconds).

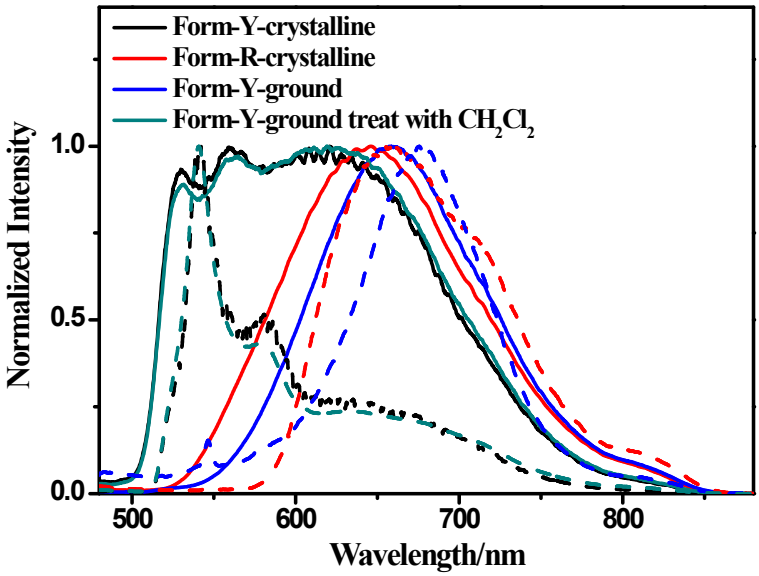

Fig. S7 Emission spectra of (+)-**1** with different solid-state forms as well as in the reversible mechanochromic process at room temperature (solid line) and 77 K (dash line) (Amorphous solid: crystallites of **Form-Y** after grinding for tens of seconds; λ_{ex} = 450 nm).

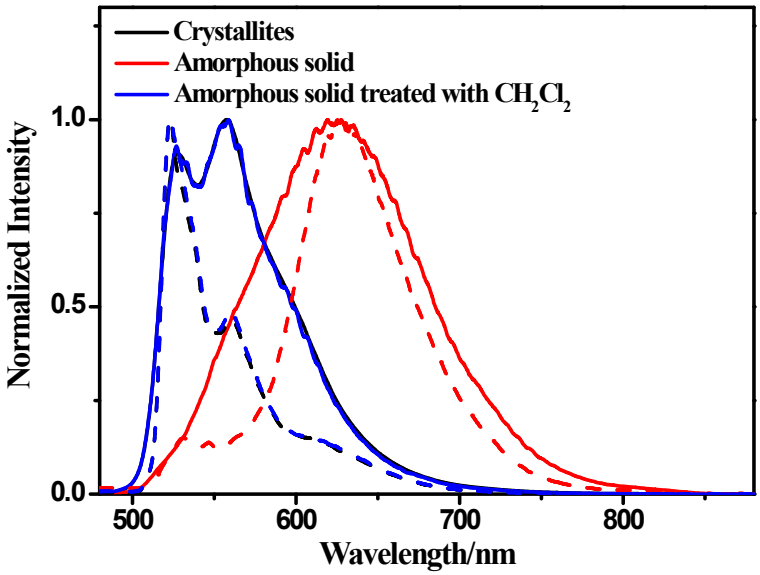

Fig. S8 Emission spectra of green-yellow crystals of (+)-**2** as well as in the reversible mechanochromic process at room temperature (solid line) and 77 K (dash line) (Amorphous solid: crystallites of (+)-**2** after grinding for tens of seconds; λ_{ex} = 450 nm)

Table S1 Crystallographic data of (−)-**1-Form-R** and (−)-**2**.

	(−)-**1-Form-R**	(−)-**2**
Formula	$C_{68}H_{82}Cl_2N_6O_7Pt_2$	$C_{66}H_{59}F_6N_6O_6S_2Pt_2$
Mr/g mol^{-1}	1556.48	1600.49
crystal system	Trigonal	Triclinic
Space group	$P3_121$	$P1$
a/Å	31.521(3)	9.895(2)
b/Å	31.521(3)	11.075(2)
c/Å	7.118(2)	15.169(3)
α/ °	90.00	71.726(3)
β/ °	90.00	83.896(4)
γ/ °	120	85.526(4)
V/Å^3	6124.8(19)	1567.8(6)
Z	3	1
T /K	291(2)	296(2)
Radiation, *λ* /Å	0.71073	0.71073
D_{calcd}, g/cm^{-3}	1.266	1.695
μ/mm^{-1}	3.533	4.598
F(000)	2334	787
Crystal size/mm^3	0.28×0.24×0.22	0.28×0.20×0.13
θ range/°	0.75 to 27.50	1.42 to 26.00
Reflections measured	56494	9516
Unique reflections	9397	7612
R_{int}	0.0785	0.0337
Reflections with $F^2 > 2\sigma(F^2)$	7499	6437
Number of parameters	459	729
Goodness-of-fit on F^2	1.048	1.054
R_1 [$F^2 > 2\sigma(F^2)$]	0.0632	0.0645
wR_2 (all data)	0.1741	0.1734
$\Delta\rho_{max}$, $\Delta\rho_{min}$ /e Å^{-3}	6.945, -6.043	2.208, -1.487

Table S2 Structural parameters of both solid-state forms of complexes (−)-**1** as well as yellow crystals of (−)-**2** determined by X-ray single crystal diffraction.

Bond Length	(−)-**1**-**Form-Y**	(−)-**1**-**Form-R**	(−)-**2**
Pt1−C1	2.018(15)	1.861(12)	2.081(6)
Pt1−C2	1.87(3)	2.088(11)	2.076(17)
Pt1−N1	1.915(15)	1.884(9)	1.929(8)
Pt1−N2	2.12(3)	2.135(9)	2.163(12)
Pt2−C3	2.016(10)		1.933(13)
Pt2−C4	1.86(3)		1.800(15)
Pt2−N3	1.923(9)		1.957(8)
Pt1−N4	2.106(8)		2.099(7)
Bond Angles	(−)-**1**-**Form-Y**	(−)-**1**-**Form-R**	(−)-**2**
C1−Pt1−C2	97.7(13)	92.9(5)	91.5(5)
C1−Pt1−N1	81.5(9)	175.3(4)	83.6(3)
C1−Pt1−N2	160.1(10)	104.7(4)	161.0(4)
C2−Pt1−N1	177.6(12)	83.3(4)	173.0(5)
C2−Pt1−N2	102.1(15)	162.3(4)	107.5(5)
N1−Pt1−N2	78.7(10)	79.0(4)	77.5(4)
C3−Pt2−C4	96.6(14)		102.8(7)
C3−Pt2−N3	81.9(5)		78.9(6)
C3−Pt2−N4	161.2(5)		157.2(6)
C4−Pt2−N3	178.2(13)		177.4(5)
C4−Pt2−N4	102.1(14)		100.0(5)
N3−Pt2−N4	79.4(3)		78.4(3)