Two segregated columnar stack platinum-bis-dithiolene molecule solids showing spin-Peierls-type transition above room temperature

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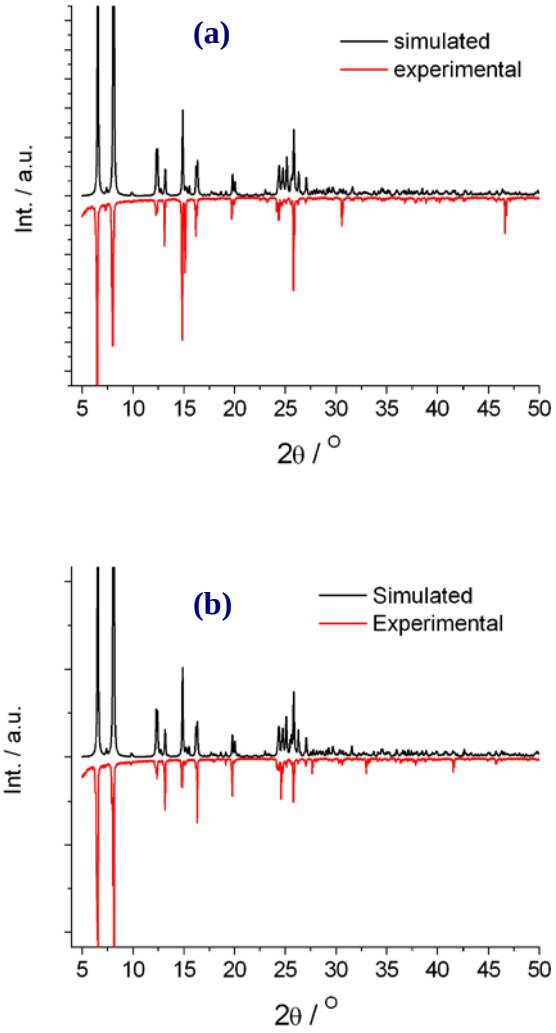
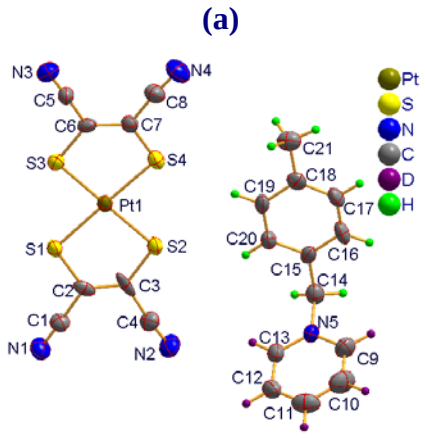


Figure S1 PXRD plots of (a) **1** and (b) **2** (red lines: experimental profiles and black lines: simulated profiles).



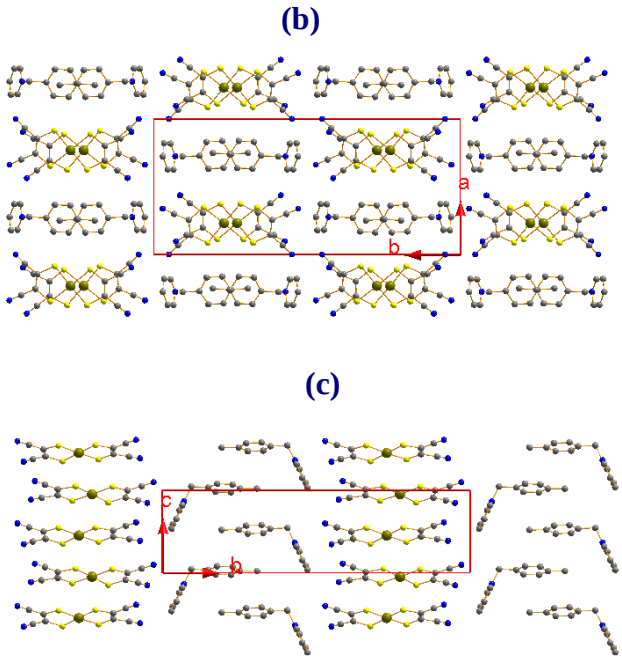


Figure S2 (a) Molecular structure with non-hydrogen atoms labeling and displacement ellipsoids at the 20% probability (b) packing diagrams of **2** viewed respectively along *c*- and *a*-axis, which shows segregated columnar stacks of anion and cation as well as alignment patterns of the neighboring superimposed anions within an anionic stack and overlapped cations within a cationic stack in HT phase.

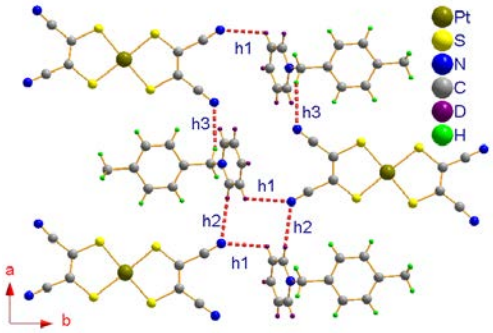
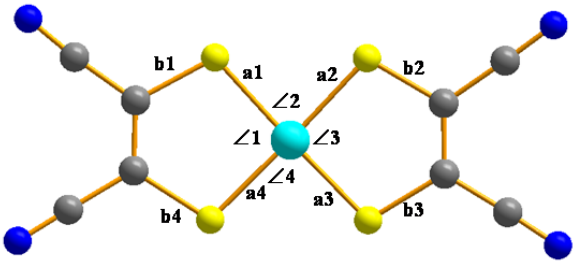


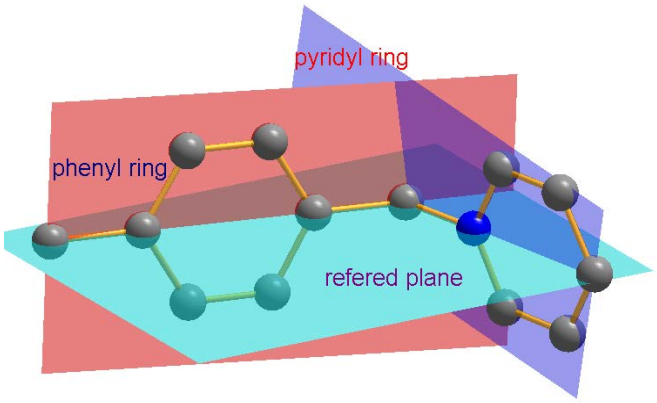
Figure S3 Characteristic H…N distances between anion and cation stacks in HT phase of **2**.

Table S1: Characteristic bond lengths (Å) and angles (°) in $[Pt(mnt)_2]^-$ moiety of **1** and **2**



	1		**2**	
	296 K		296 K	
	With Pt1	With Pt2	With Pt1	With Pt2
∠1	90.1(3)	90.3(3)	92.23(6)	92.32(7)
∠2	88.6(3)	88.6(3)	92.38(6)	92.42(7)
∠3	89.5(3)	90.0(3)	87.62(6)	87.45(6)
∠4	91.7(3)	91.2(3)	87.80(6)	87.83(6)
a1	2.248(9)	2.243(9)	2.248(5)	2.250(6)
a2	2.272(9)	2.249(8)	2.274(5)	2.253(5)
a3	2.239(9)	2.264(9)	2.252(5)	2.259(5)
a4	2.260(8)	2.272(10)	2.263(5)	2.269(6)
b1	1.74(4)	1.71(4)	1.72(2)	1.70(2)
b2	1.75(3)	1.71(3)	1.73(2)	1.710(19)
b3	1.74(5)	1.73(4)	1.73(2)	1.72(2)
b4	1.68(3)	1.71(4)	1.71(2)	1.72(2)
	353 K		353 K	
	With Pt1		With Pt1	
∠1	89.72(7)		89.63(11)	
∠2	91.74(7)		91.80(11)	
∠3	89.73(7)		89.59(11)	
∠4	88.82(7)		88.99(11)	
a1	2.256(2)		2.264(3)	
a2	2.2598(19)		2.266(3)	
a3	2.2658(19)		2.276(3)	
a4	2.2718(19)		2.266(3)	
b1	1.726(7)		1.751(12)	
b2	1.722(7)		1.665(11)	
b3	1.718(8)		1.721(12)	
b4	1.703(8)		1.691(11)	

Table S2: Characteristic dihedral angles (°) in cations of **1** and **2**



	1		**2**	
	296 K		296 K	
∠*1*	82.14	84.09	82.99	85.45
∠*2*	88.57	87.05	87.47	84.43
∠*3*	67.54	71.59	66.68	70.74
	353 K		353 K	
∠*1*	85.39		84.55	
∠*2*	86.24		85.93	
∠*3*	67.94		67.89	

Notes: ∠*1*, ∠*2* and ∠*3* represent the dihedral angles between phenyl ring and referred plane, between phenyl ring and the referred plane as well between phenyl ring and pyridyl ring (there are two crystallographically different cations in LT phase).