Electronic Supplementary Material (ESI) for Dalton Transactions.

Spin crossover phenomenon in a 2D heterometallic coordination polymer with $[Pd(SCN)_4]^{2-}$ building blocks

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Table S1. π···π interactions between anthracene units in **1** and **2**.

	1		**2**
	120 K	**298 K**	**150 K**
Z^a	5.7464(3)	5.7286(5)	5.8262(2)
Z^b	4.8131(2)	4.8992(4)	4.7646(2)
l^c	2.5762(1)	2.6528(2)	3.4516(2)
r^d	0.47628	0.48534	0.61034
θ^e	67.106(113)	68.946(244)	36.719(163)
α^f	156.097(2)	161.855(4)	108.942(2)

[a]The distance between the centroids of anthracene rings (Å); [b]The shortest distance between the centroids of benzene rings (Å); [c]The shortest distance of H-to-ring center (Å); [d]The offset distance between two aromatic rings (Å); [e]The angle between two aromatic rings (°); [f]The angle of π–H ··· π (°).

Table S2. π···π interactions between anthracene and pyridine units in **1** and **2**.

		Z^c	l^d	r^e	θ^f
1_120 K	anth1 and py1[a]	5.1557(3)	2.9655(11)	0.5115	67.009(138)
1_298 K	anth1 and py1[a]	5.2495(6)	3.0354(3)	0.5210	70.504(227)
2_150 K	anth1 and py1[b]	4.6187(2)	2.9100(1)	1.3887	53.082(236)
	anth2 and py1[b]	4.6627(2)	2.5864(1)	1.3887	53.082(241)

[a]anth1: C7-C12, x, 1+y, z; py1: C1-C5, N1, x, y, z.
[b]anth1: C7-C12, 3/2-x, -1/2+y, 1/2-z, z; py1: C1-C5, N1, x, y, z; anth2: C7-C12, x, y, z, py1: C1-C5, N1, 3/2-x, -1/2+y, 1/2-z.
[c]The shortest distance between the centroids of aromtic rings (Å); [d]The shortest distance of H-to-ring center (Å); [e]The offset distance between two aromatic rings (Å); [f]The angle between two aromatic rings (°)

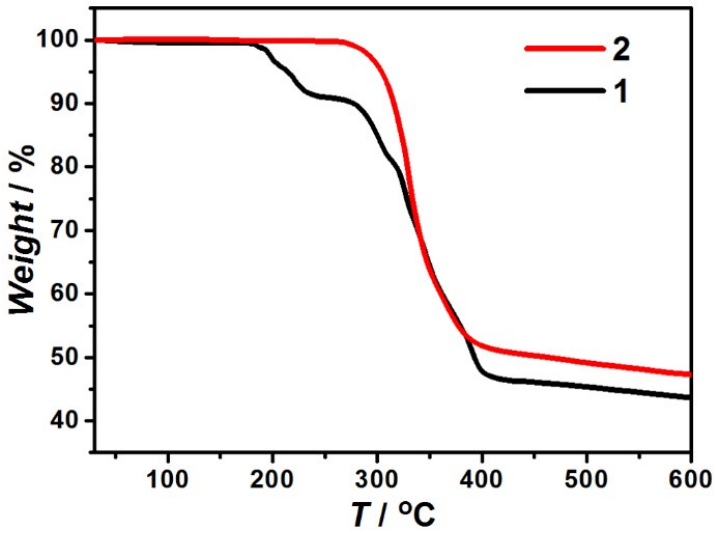

Figure S1. Thermogravimetric analyses of **1** and **2**.

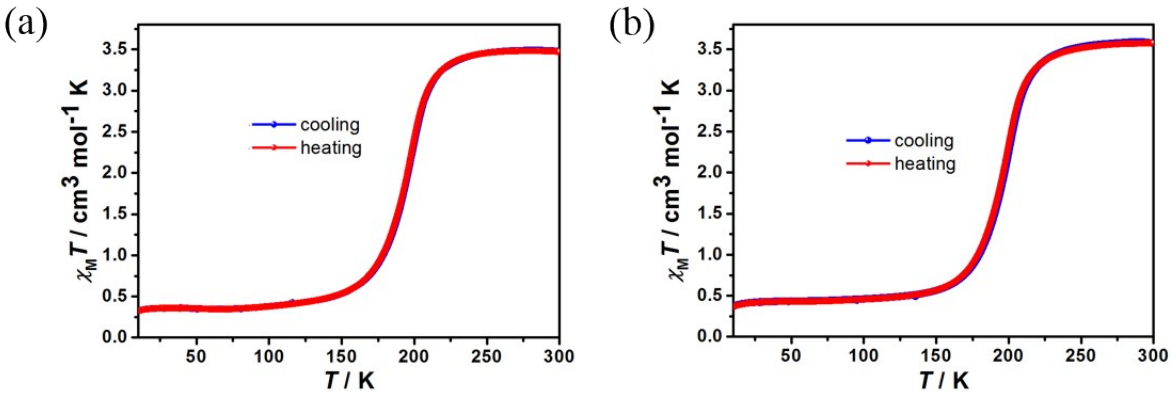

Figure S2. Magnetic susceptibility data for **1** at 2 K min^{-1} on fresh samples (a) and 0.5 K min^{-1} on old samples (aged about one year) (b) in the cooling and warming modes.

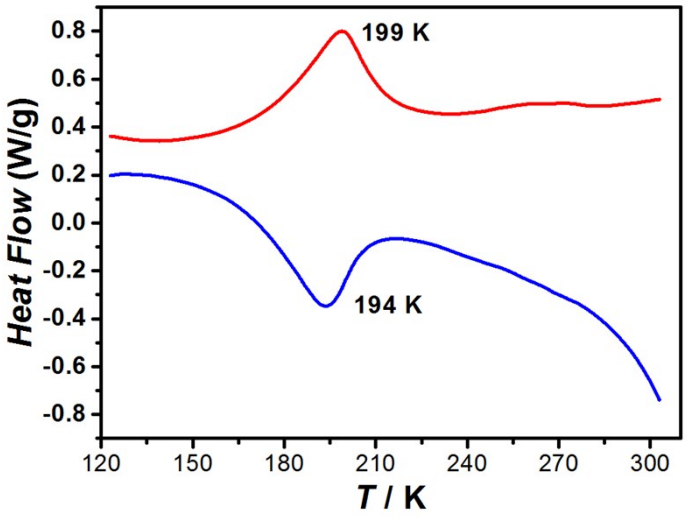

Figure S3. Differential scanning calorimetry (DSC) measurements of **1**.

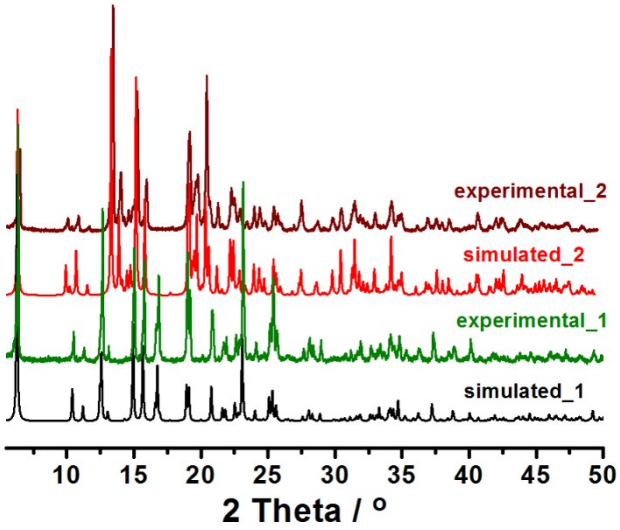

Figure S4. Powder X-ray diffraction data of **1** and **2**.

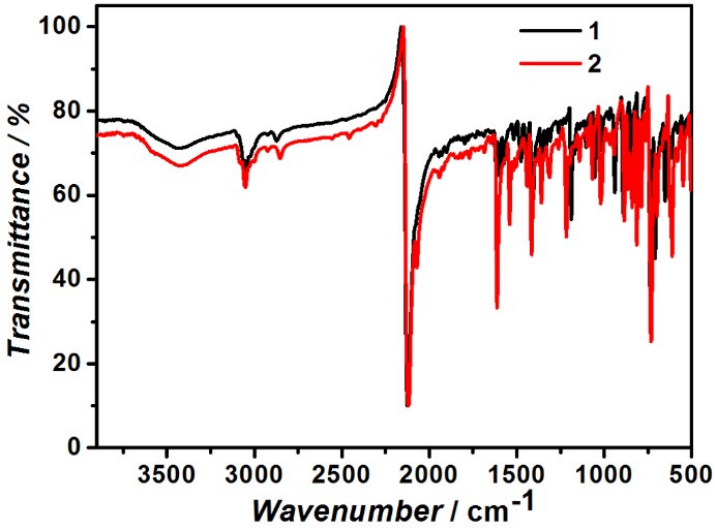

Figure S5. IR spectra of **1** and **2**.

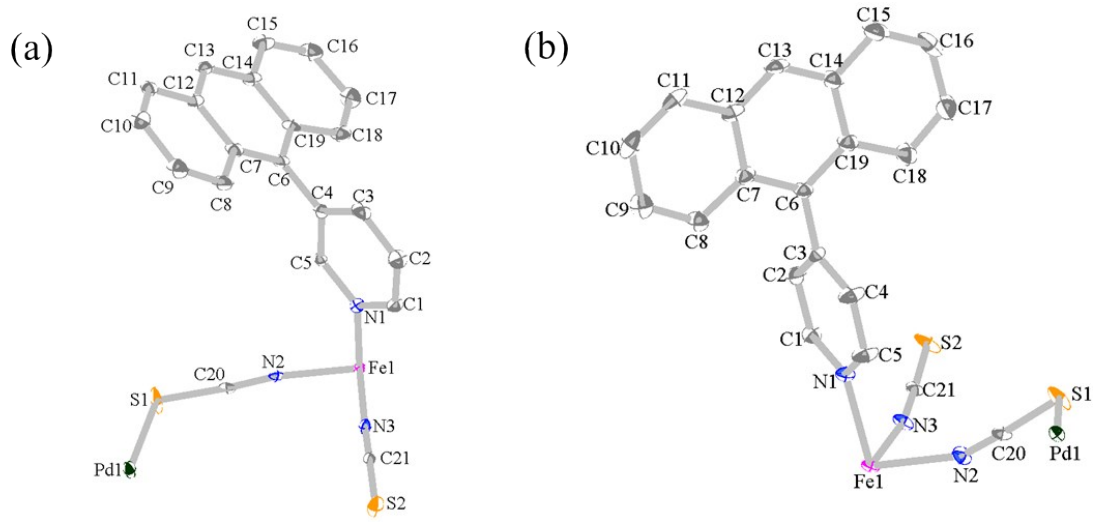

Figure S6. Asymmetric units of **1** (a) and **2** (b). Hydrogen atoms are omitted for clarity.

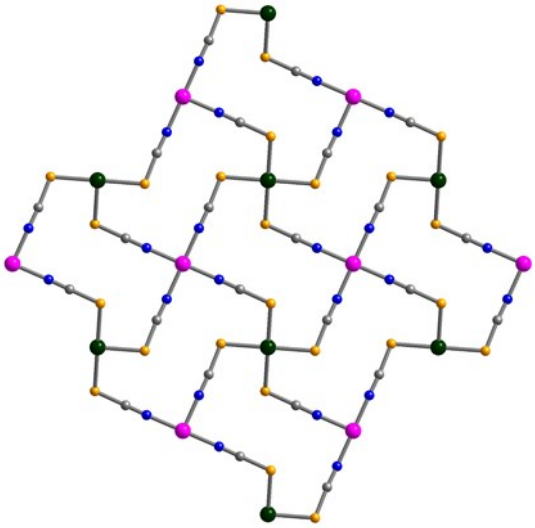

Figure S7. Top view of the two-dimensional coordination layer in **1** at 120 K.

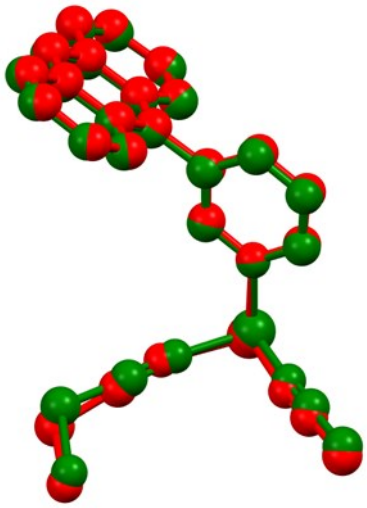

Figure S8. The overlaid structures of **1**: green (LS), red (HS). Hydrogen atoms are omitted for clarity.