Electronic Supplementary Material (ESI) for Dalton Transactions

Observation of metal ion dependent packing structures and magnetic behaviors of metal-bis-1, 2-dithiolene complexes

Wen-Bo Pei [a] Jian-Sheng Wu [a] Xiao-Ming Ren *[a,b] Zheng-Fang Tian [a] Jingli Xie *[c]

[a] State Key Laboratory of Materials-Oriented Chemical Engineering and College of Science, Nanjing University of Technology, Nanjing 210009, P. R. China

[b] State Key Lab & Coordination Chemistry Institute, Nanjing University, Nanjing 210093, P. R. China

[c] School of Chemistry, Monash University, Clayton, Victoria 3800, Australia

Tel.: +86 25 83587820

Fax: +86 25 83587420

Email: xmren@njut.edu.cn

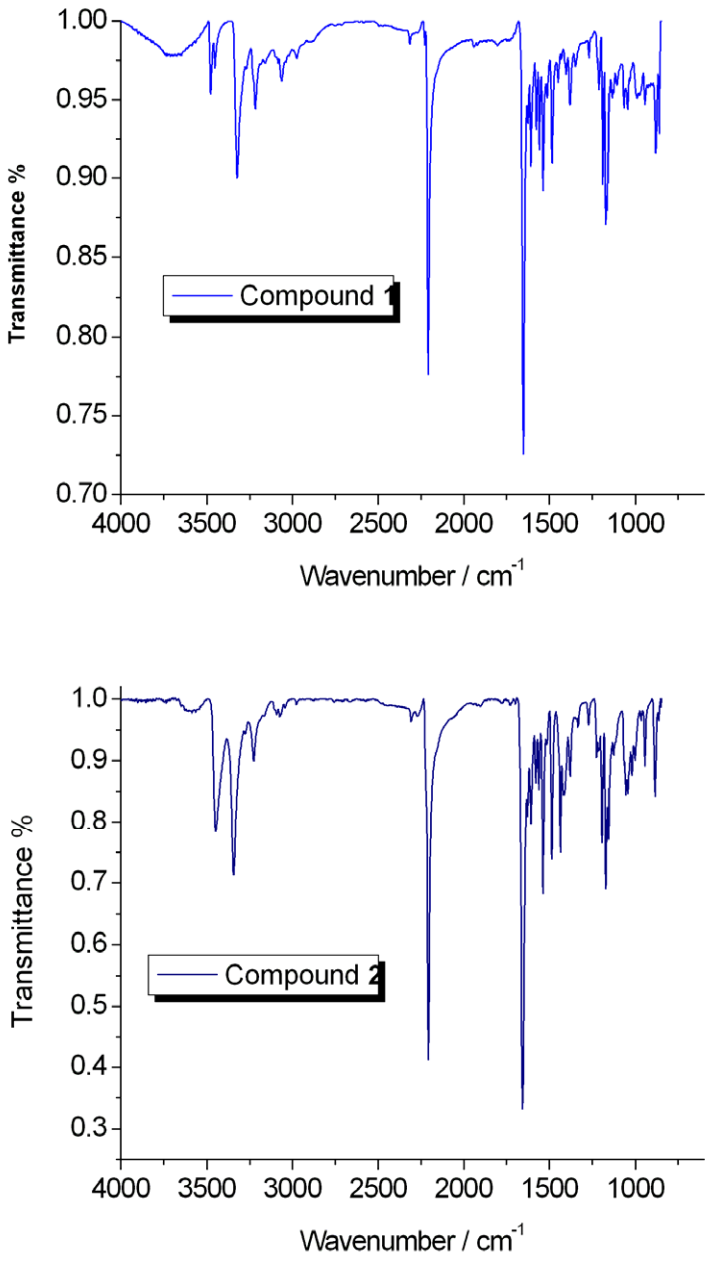

Fig. S1. FT-IR spectra of compounds **1** and **2**.

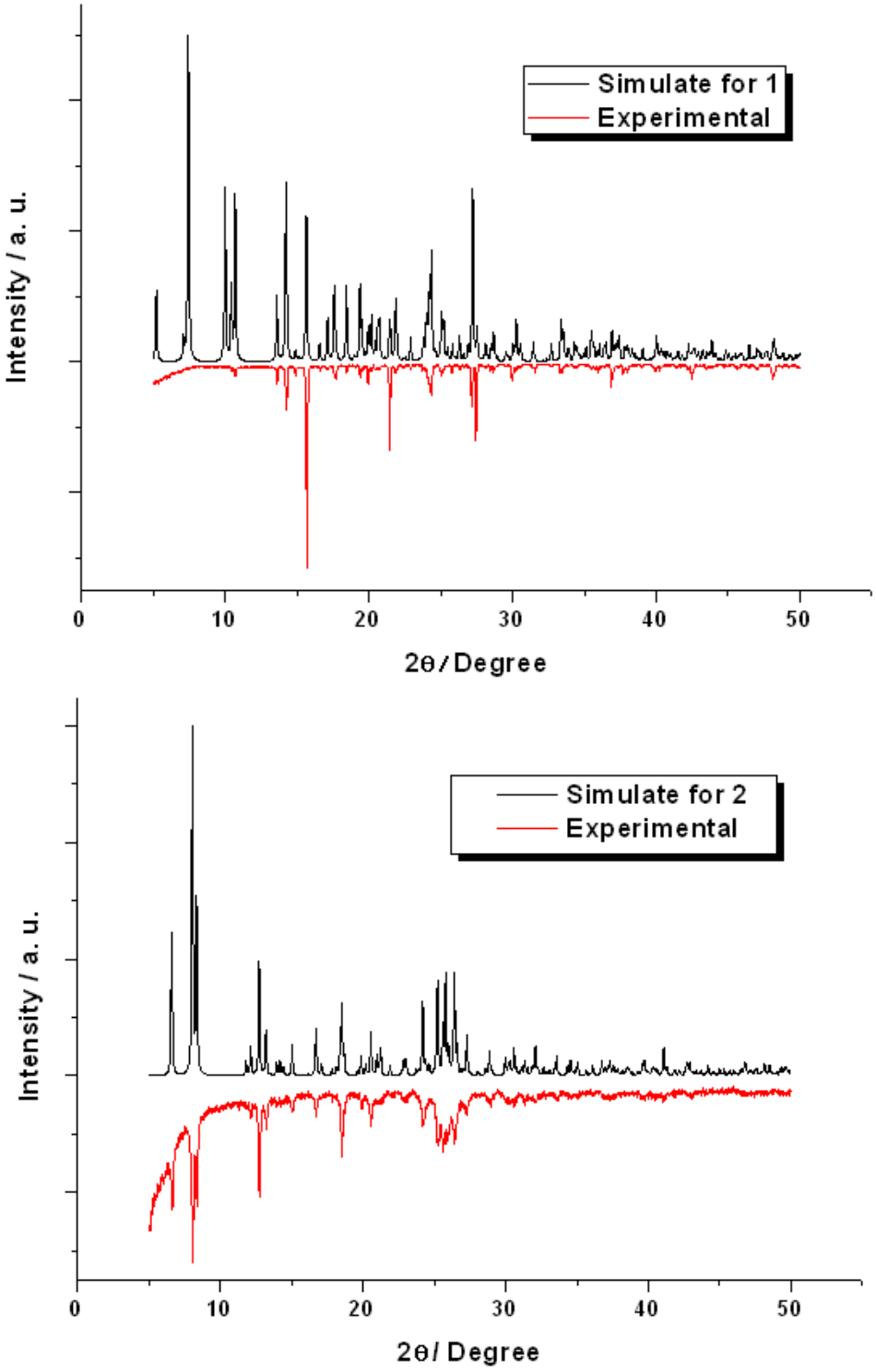

Fig. S2 Experimental and simulated X-ray powder diffraction patterns of **1** and **2**.

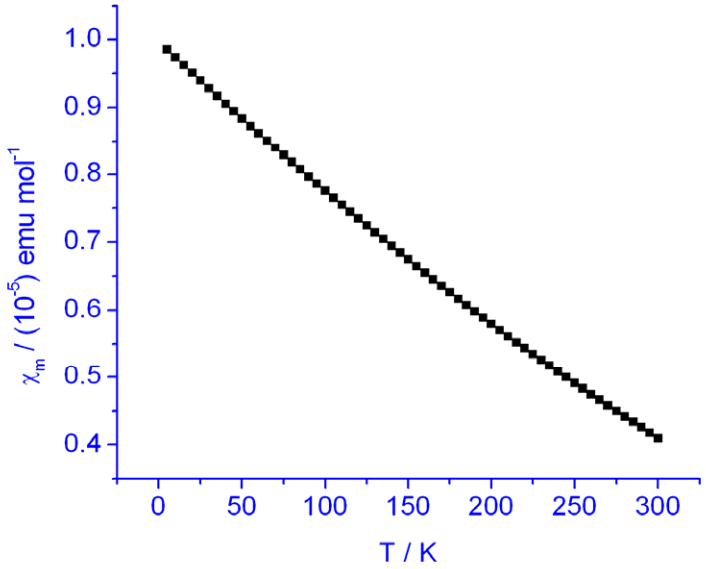

Fig. S3 The reproduced molar magnetic susceptibility of **2** using the magnetic susceptibility expression of the S = ½ Heisenberg alternating chain with the alternating constant α = 0.08 and J/k_B = 4103 K from DFT calculation. The paramagnetic susceptibility contributed from the spin chain is less 3% of that the experimental molar magnetic susceptibility in the temperature range of 50-300 K.

Table S1 The calculated $<S^2>_{HS}$, $<S^2>_{BS}$ and J values for each spin dimer in the crystals of **1** and **2** at ubp86/lanl2dz, ub3lyp/lanl2dz and usvwn/lanl2dz levels

Complex	Spin dimer	$J^{(1)}/k_B$ (K)	$J^{(2)}/k_B$ (K)	$J^{(3)}/k_B$ (K)	$<S^2>_{HS}$	$<S^2>_{BS}$
			ubp86/lanl2dz			
1	J_1	-45	-22	-44	2.0035	0.9743
2	J_1**	-7404	-3702	-3696	2.0033	0.0000
	J_2**	-62	-31	-31	2.0032	0.0000
			ub3lyp/lanl2dz			
1	J_1	-12	-6	-12	2.0140	1.0101
2	J_1**	-5414	-2707	-2688	2.0144	0.0000
	J_2**	2659	1329	1321	2.0135	0.0000
			usvwn/lanl2dz			
1	J_1	692	346	346	2.00022	0.0000
2	J_1**	-8179	-4090	-4085	2.0021	0.0000
	J_2**	-501	-250	-250	2.0020	0.0000

**J_1 and J_2 correspond to the $[Pd(mnt)_2]_2^{2-}$ dimers with $d_{Pd...Pd}$ = 3.408 and 4.385 Å, respectively