Electronic Supplementary Material (ESI) for New Journal of Chemistry

Two magnetic phase transition driven respectively by symmetry breaking and isostructural phase transitions in a nickel-bis-dithiolene spin system

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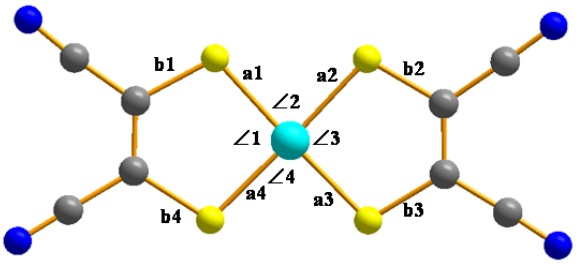
Table S1: Characteristic bond lengths (Å) and angles (°) in $[Ni(mnt)_2]^-$ moiety



	200 K (α phase)		296 K (β phase)	353 K (γ phase)
	With Ni1	With Ni2		
∠1	92.57(4)	92.57(4)	92.23(6)	92.32(7)
∠2	92.90(4)	92.61(4)	92.39(6)	92.43(7)
∠3	87.64(4)	87.92(4)	87.61(6)	87.44(6)
∠4	86.82(4)	87.34(4)	87.80(6)	87.82(6)
a1	2.1451(10)	2.1500(11)	2.1311(15)	2.1373(16)
a2	2.1457(11)	2.1500(11)	2.1409(16)	2.1405(17)
a3	2.1500(10)	2.1518(11)	2.1413(16)	2.1412(17)
a4	2.1554(10)	2.1539(11)	2.1428(16)	2.1474(17)
b1	1.719(4)	1.715(4)	1.715(5)	1.698(6)
b2	1.710(4)	1.718(4)	1.719(6)	1.716(6)
b3	1.712(4)	1.724(4)	1.714(5)	1.696(6)
b4	1.719(4)	1.714(4)	1.723(6)	1.709(6)

Table S2: The equivalent displacement parameters (U_{eq}) and the ratios for the same atoms at different temperatures as compared with 296 K

Non-hydrogen atom	U_{eq}(353 K) in γ phase	U_{eq}(296 K) in β phase	U_{eq}(353 K)/U_{eq}(296K)
Ni1	0.0828(4)	0.0728(3)	1.137
S1	0.0953(5)	0.0835(4)	1.141
S2	0.0893(5)	0.0775(4)	1.152
S3	0.1008(5)	0.0943(5)	1.069
S4	0.0903(5)	0.0825(4)	1.095
N1	0.152(3)	0.140(2)	1.086
N2	0.161(3)	0.142(2)	1.134
N3	0.154(3)	0.150(2)	1.027
N4	0.127(2)	0.125(2)	1.016
N5	0.140(2)	0.131(2)	1.069
N6	0.173(3)	0.180(4)	0.929
C1	0.112(2)	0.0971(17)	1.153
C2	0.0920(16)	0.0774(13)	1.189
C3	0.0828(15)	0.0726(13)	1.140
C4	0.111(2)	0.0950(16)	1.169
C5	0.117(2)	0.1093(19)	1.070
C6	0.0921(16)	0.0896(16)	1.028
C7	0.0856(16)	0.0833(15)	1.028
C8	0.0973(18)	0.0967(17)	1.006
C9	0.155(3)	0.154(3)	1.006
C10	0.148(3)	0.151(3)	0.961
C11	0.159(3)	0.175(4)	0.909
C12	0.156(3)	0.147(3)	1.061
C13	0.162(4)	0.139(3)	1.165
C14	0.299(9)	0.264(8)	1.133
C15	0.151(3)	0.165(4)	0.915
C16	0.144(3)	0.118(2)	1.22

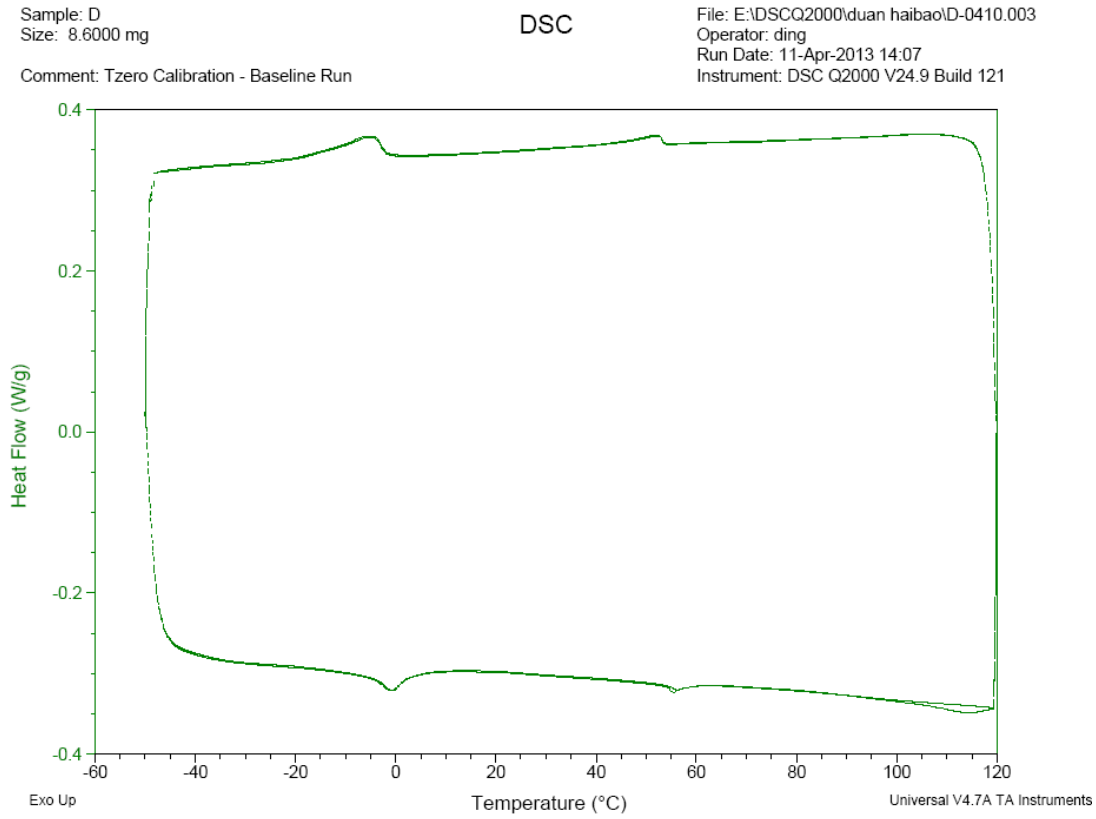


Figure S1 DSC plot of **1**.