

Supporting Information

Construction of three high-dimensional supramolecular networks from temperature-driven conformational isomers[†]

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Materials and physical measurements: All reagents were commercially available and used without further purification. Infrared spectra were obtained from KBr pellets on a Bruker TENSOR 27 Fourier transformation infrared spectrometer in the 400-4000 cm⁻¹ region. Elemental analyses (C, H, N) were performed on a Perkin-Elmer 240 elemental analyzer. Powder X-ray diffraction (PXRD) data were recorded on a Rigaku D/M-2200T automated diffractometer. The luminescent spectra for the solid state were recorded at room temperature on an Aminco Bowman Series 2 spectrofluorometer with a xenon arc lamp as the light source. In the measurements of emission and excitation spectra the pass width is 5.0 nm.

Table S1 Distances (Å) and angles (°) of hydrogen bonds for the compounds **1-3**.

D-H···A	d(H···A)	d(D···A)	∠D-H···A
α-1			
C(2)-H(2)···N(6)#1	2.654(6)	3.457(5)	145(2)
C(3)-H(3)···N(6)#1	2.717(5)	3.530(5)	167(2)
C(6)-H(6)···N(4)#2	2.695(5)	3.528(5)	150(2)
C(2)-H(2)···N(6)#3	2.654(6)	3.457(6)	145(3)
C(7)-H(7A)···N(6)#4	2.699(5)	3.502(5)	141(2)
π···π	3.606(5)		
β-2			
C(3)-H(3)···N(9)#4	2.588(4)	3.460(4)	156(2)
C(6)-H(6)···N(6)#4	2.612(4)	3.456(5)	151(2)
C(7)-H(7A)···N(6)#5	2.739(3)	3.584(4)	146(2)
C(8)-H(8B)···N(9)#6	2.623(4)	3.546(4)	159(2)
C(9)-H(9B)···π	3.178(4)		
γ-3			
C(3)-H(3)···N(6)#7	2.704(5)	3.390(5)	131(2)
C(2)-H(2)···N(6)#7	2.700(5)	3.329(5)	126(2)
C(10)-H(10)···π	3.052(5)		

*Symmetry transformation used to generate equivalent atoms: #1 x,1+y,z; #2 1+x,y,z;
#3 x,y-1,z+1; #4 x,y,1+z; #5 1+x,y,1+z; #6 1-x,-y,-z; #7 x,1+y,1+z.

Scheme S1. Several symmetrical-and unsymmetrical Schiff base ligands involved in text.

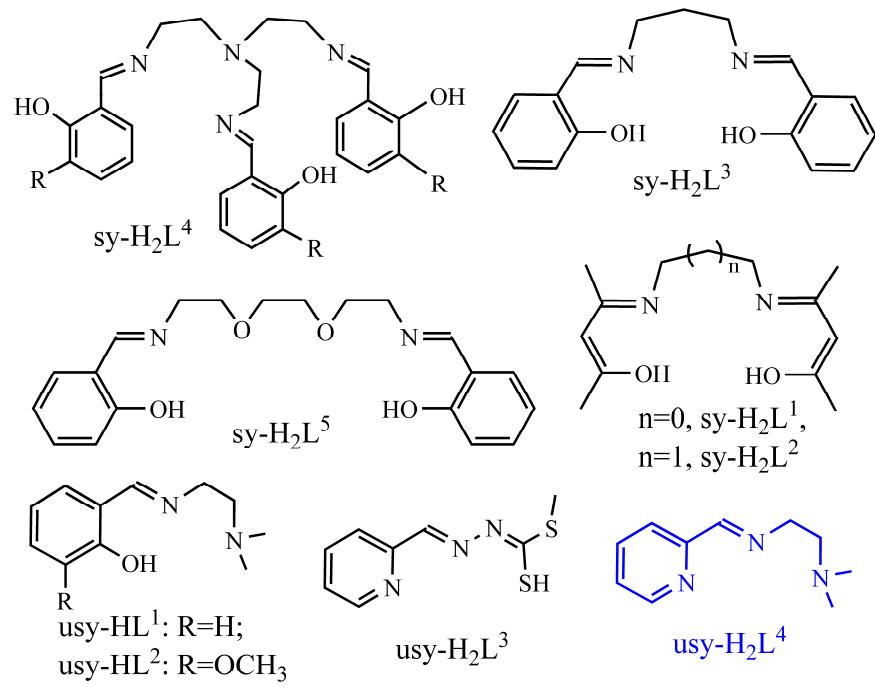


Figure S1 Molecular structure of isomer $\beta\text{-2}$ with the atom numbers. The selected bond distances Zn1-N1 2.226(3), Zn1-N2 2.067(3), Zn1-N3 2.274(4), Zn1-N4 1.977(4), Zn1-N7 1.985(4) Å.

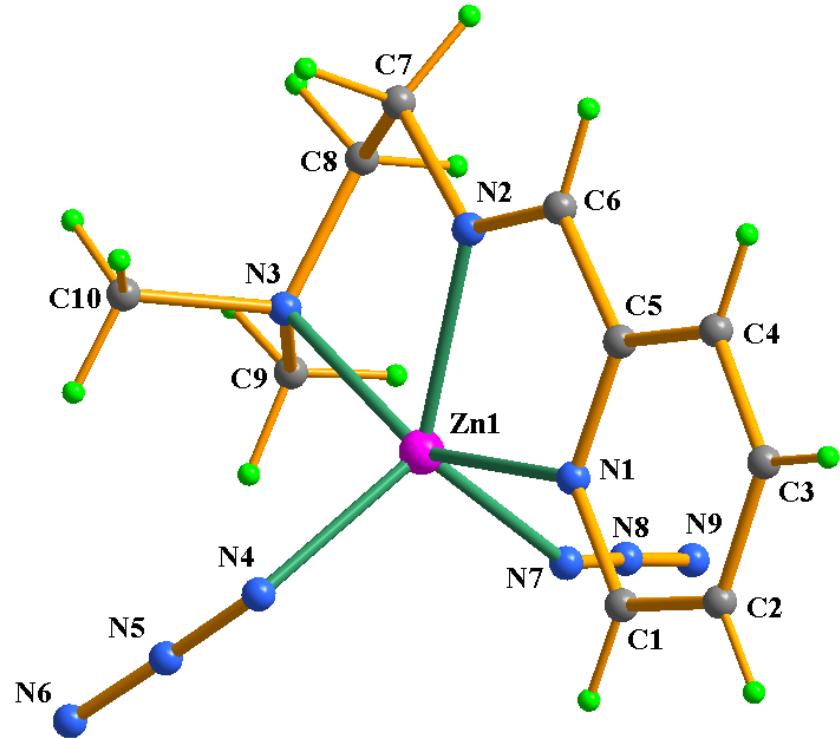


Figure S2 Molecular structure of isomer γ -3 with the atom numbers. The selected bond distances Zn1-N1 2.236(3), Zn1-N2 2.067(4), Zn1-N3 2.261(4), Zn1-N4 2.011(4), Zn1-N7 1.976(4) Å.

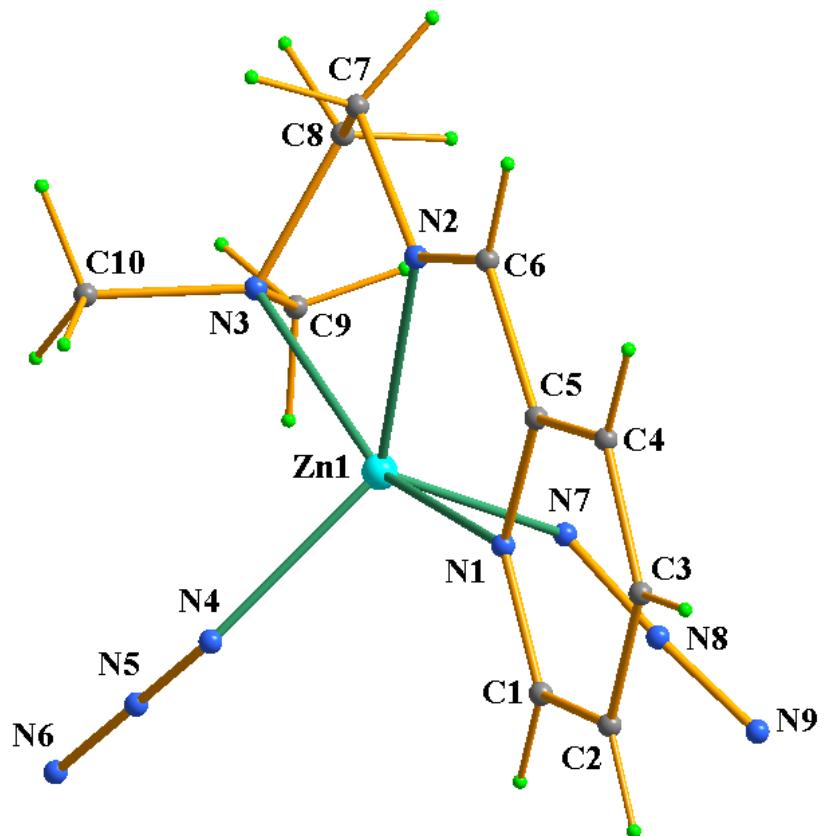


Figure S3 2-D supramolecular layer through hydrogen bonding C-H···N and $\pi\cdots\pi$ packing interactions in compound **1** along *c* axis direction.

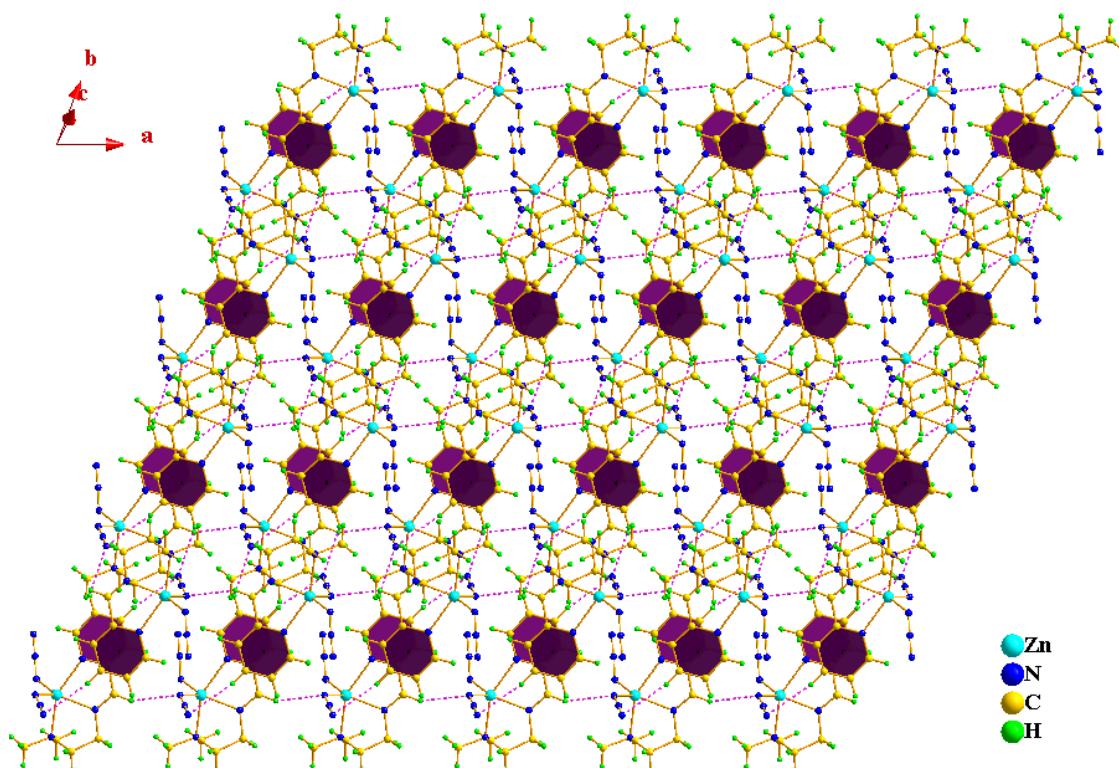


Figure S4 3-D supramolecular layer constructed through hydrogen bonding C-H…N interactions in compound **2** along *c* axis direction.

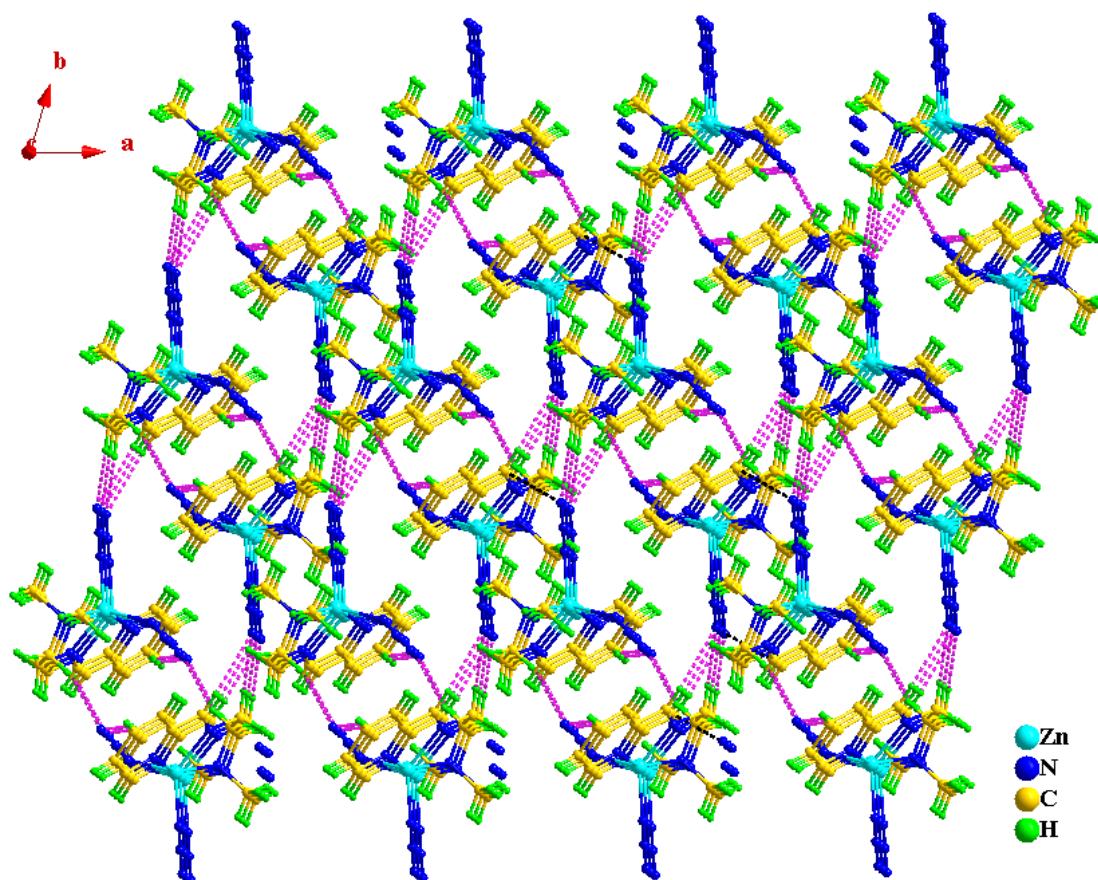


Figure S5 3-D supramolecular layer constructed through hydrogen bonding C-H···N and C-H··· π packing interactions in compound **3** along *b* axis direction.

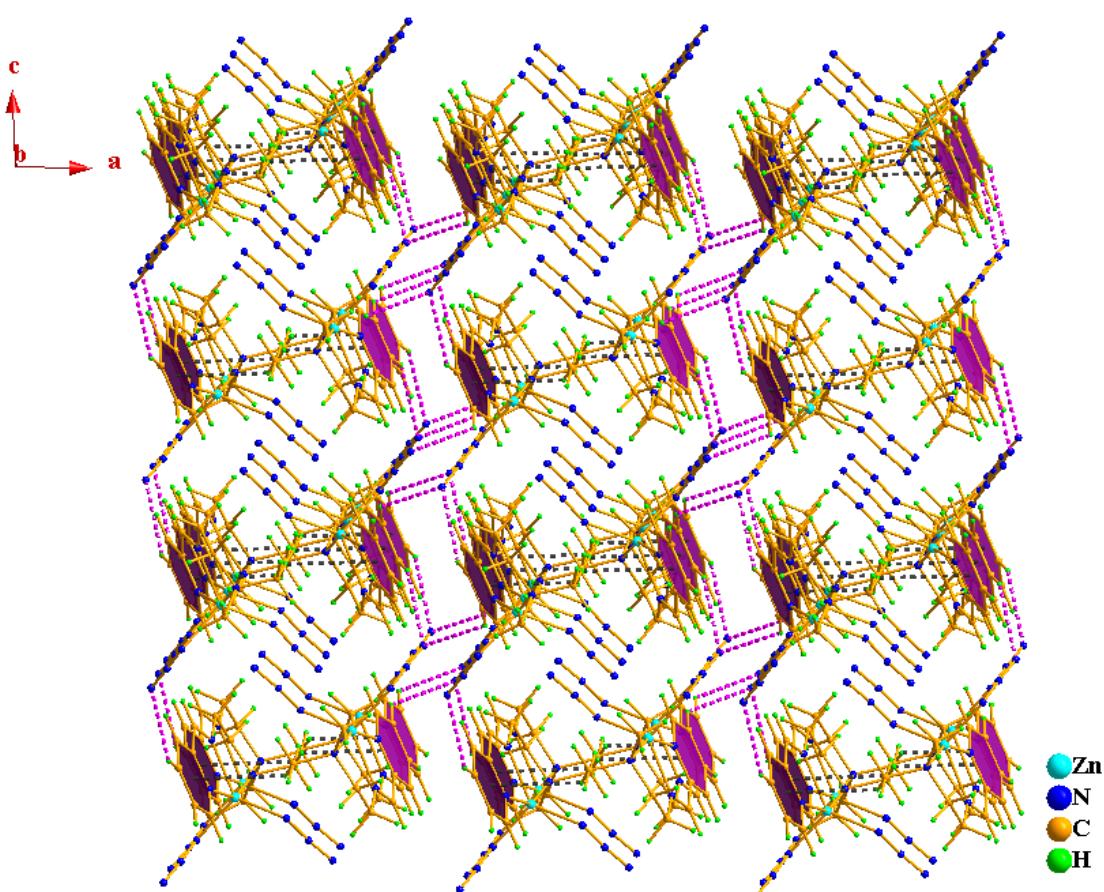
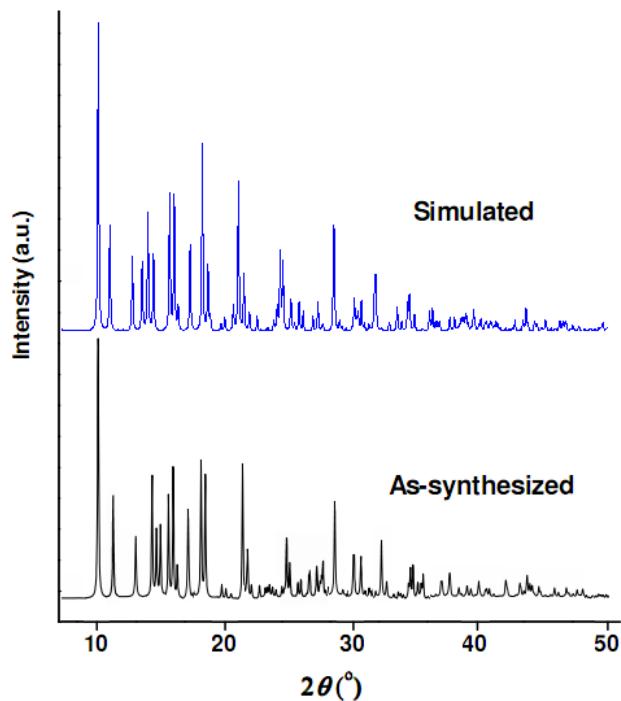
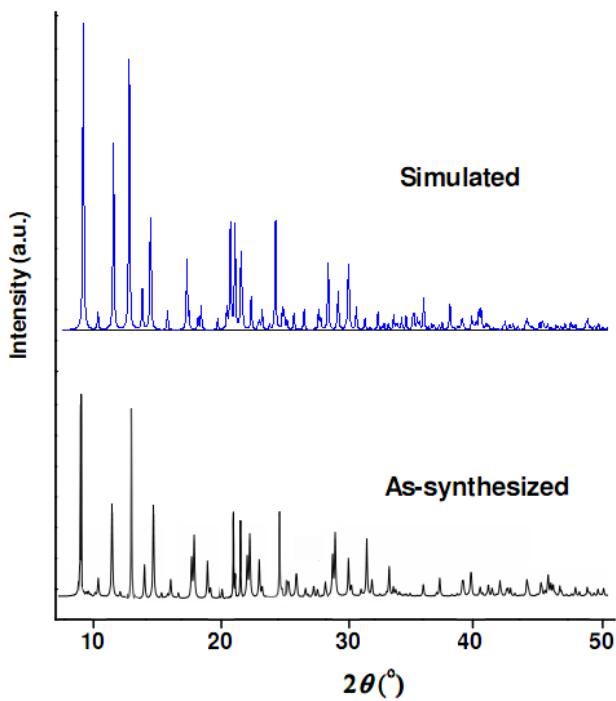


Figure S6 PXRD patterns of three compounds **1-3** simulated from the X-ray single-crystal structure and as-synthesized samples.

(1) for Compound 1



(2) for Compound 2



(3) for Compound 3

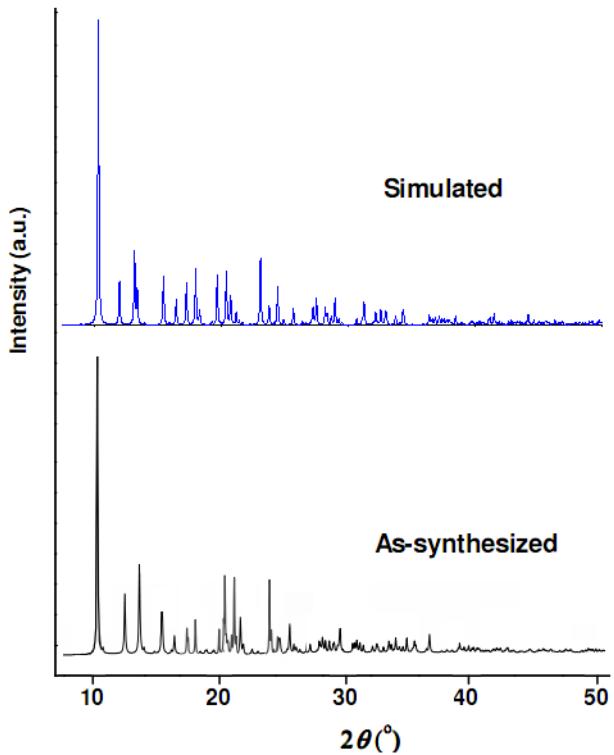
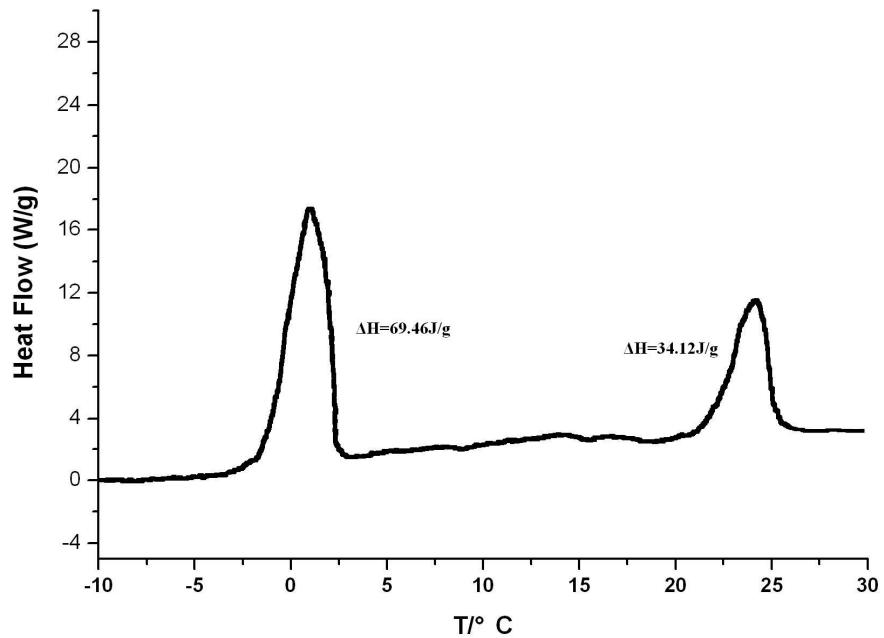


Figure S7 Two DSC curves showing (a) the heating of **1** through to **3** and then (b) the cooling of **3** through **1**.

(a)



(b)

