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RESEARCH ARTICLE

Iron(II) Spin Crossover Polymers of Planar N₂O₂ Schiff Base Templates and 4,4'-bis(pyridyl)urea Bridges

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Article History

Received: March 06, 2018

Revised: May 17, 2018

Accepted: January 27, 2019

SUPPLEMENTARY MATERIAL

In the Supporting Information, the crystallographic data of

4 and 5, an excerpt of the 1D chain of 5, the PXRD pattern of 1, 2, 4 and 5, and the magnetic properties of 1* and 5 are given.

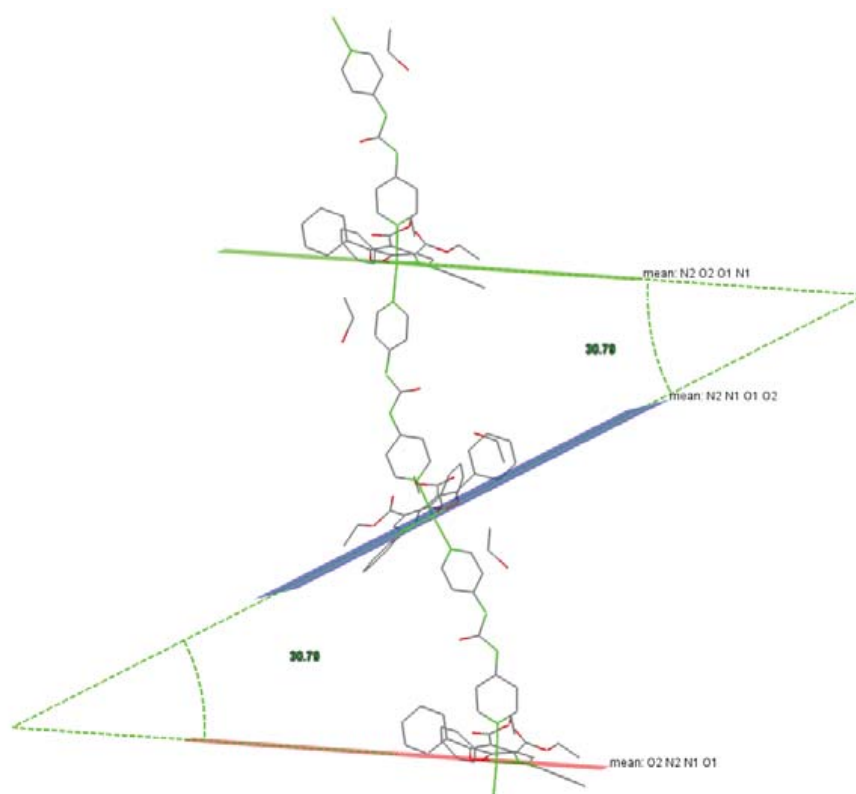


Fig. (SP1). Excerpt of the 1D chain of 5 to illustrate the relative angle between the planes of the Schiff base-like ligand, illustrated using Mercury.

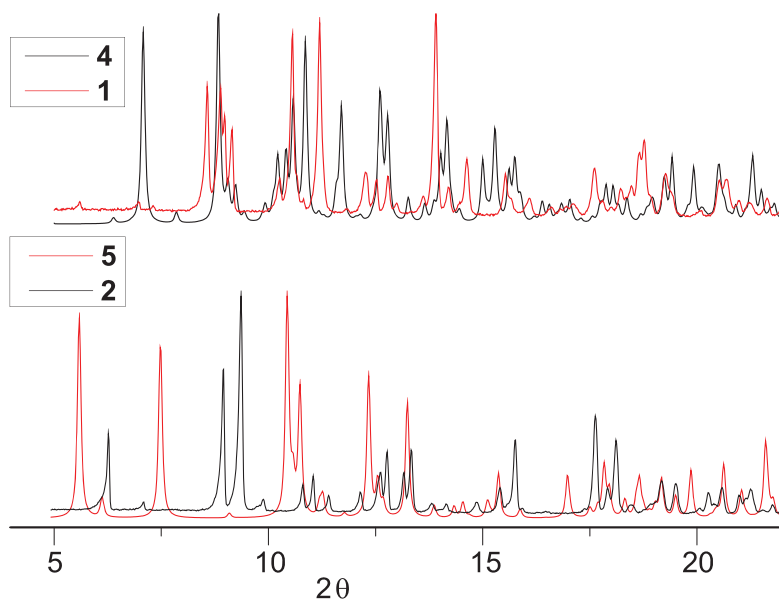


Fig. (SP2). Comparison of the calculated PXRD pattern of 4 and 5 with the measured PXRD pattern of 1 and 2.

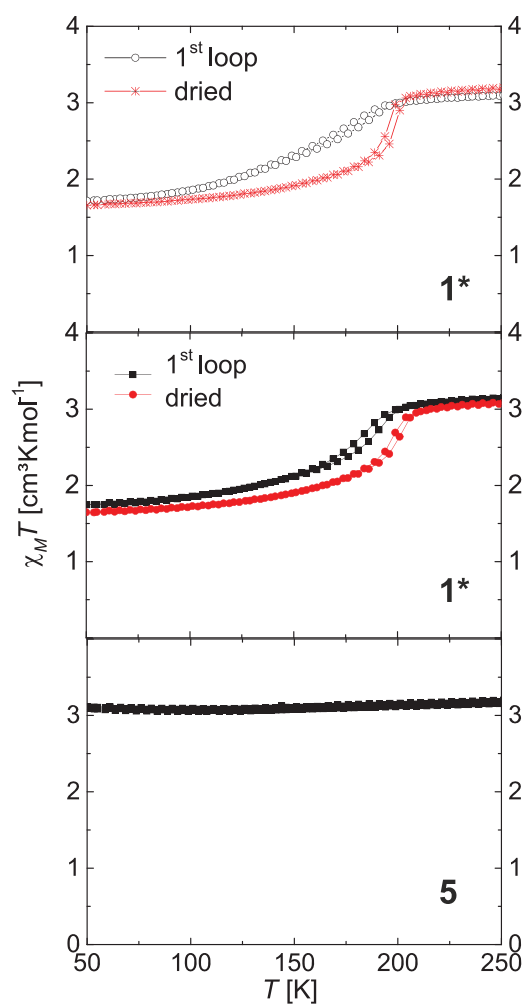


Fig. (SP3). Plot of the $\chi_M T$ product vs. T in the 250 – 50 K range for the complexes 1* and 5 discussed in this manuscript.

Table SP1. Crystallographic data of 4 and 5.

	4	5
CCDC	1827146	1827147
formula	[{Fe(L1a)(bpua)(MeOH)} ₂ -μ{Fe(L1a)}](8 MeOH)	{[Fe(L1b)(bpua)](2 EtOH)} _n
sum formula	C108 H94 Fe3 N14 O16,8(C H4 O)	C41 H36 Fe N6 O7, 2(C2 H6 O)
<i>M</i> / g mol ⁻¹	2267.85	872.74
crystal system	Triclinic	Monoclinic
space group	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>
crystal description	black block	red platelet-like
<i>a</i> / Å	10.0598(3)	15.901(2)
<i>b</i> / Å	22.7165(7)	9.9971(9)
<i>c</i> / Å	26.9491(9)	29.071(3)
<i>α</i> / °	109.743(2)	90
<i>β</i> / °	97.217(3)	100.998(8)
<i>γ</i> / °	96.984(3)	90
<i>V</i> / Å ³	5661.1(3)	4536.4(9)
<i>Z</i>	2	4
<i>ρ</i> _{calcd} / g cm ⁻³	1.331	1.278
<i>μ</i> / mm ⁻¹	0.457	0.392
crystal size /mm	0.13 x 0.13 x 0.14	0.10 x 0.14 x 0.17
F(000)	2380	1832
<i>T</i> / K	133	133
<i>λ</i> / Å	0.71069	0.71069
<i>θ</i> range/ °	1.0–28.1	1.4–28.1
Reflns. collected	62526	23052
Indep. reflns. (<i>R</i> _{int})	25363 (0.10)	10123 (0.156)
Parameters	1402	520
<i>R</i> 1 (all data)	0.0706	0.0873
<i>wR</i> 2	0.1995	0.2616
Goof	0.86	0.72