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Polymorphism and its effects on the magnetic behaviour of the [Fe(sal$_2$-trien)][Ni(dmit)$_2$] spin-crossover complex

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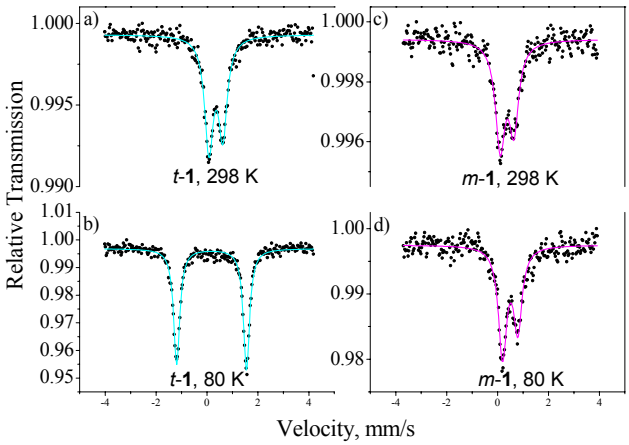

Fig. S1. Mössbauer spectra of *t*-**1** (a,b) and *m*-**1** (c,d) recorded at 298 K (a,c) and 80 K (b,d), respectively.

Table S1. Selected bond distances and bond angles with their differences in percentage at 293 K for *t*-**1** and 295 K for *m*-**1**

	t-**1**	*m*-**1**	Δ (%)
Fe(1)-O(1)	1.899(2)	1.902(2)	0.16
Fe(1)-O(2)	1.919(2)	1.896(2)	-1.20
Fe(1)-N(1)	2.118(3)	2.108(2)	-0.47
Fe(1)-N(4)	2.124(3)	2.104(2)	-0.94
Fe(1)-N(3)	2.186(3)	2.176(2)	-0.46
Fe(1)-N(2)	2.191(3)	2.193(2)	0.09
O(1)-Fe(1)-O(2)	105.1(1)	103.19(8)	-1.82
O(1)-Fe(1)-N(1)	86.9(1)	87.73(8)	0.96
O(2)-Fe(1)-N(1)	94.0(1)	91.73(8)	-2.41
O(1)-Fe(1)-N(4)	94.2(1)	100.78(7)	6.99
O(2)-Fe(1)-N(4)	86.9(1)	87.50(8)	0.69
N(1)-Fe(1)-N(4)	178.3(1)	171.41(8)	-3.86
O(1)-Fe(1)-N(3)	92.8(1)	90.83(8)	-2.12
O(2)-Fe(1)-N(3)	155.7(1)	160.42(8)	3.03
N(1)-Fe(1)-N(3)	103.4(1)	102.57(8)	-0.80
N(4)-Fe(1)-N(3)	75.3(1)	76.35(8)	1.39
O(1)-Fe(1)-N(2)	159.0(1)	157.70(8)	-0.82
O(2)-Fe(1)-N(2)	89.8(1)	92.87(8)	3.42
N(1)-Fe(1)-N(2)	77.1(1)	76.27(8)	-1.08
N(4)-Fe(1)-N(2)	101.4(1)	95.22(8)	-6.09
N(3)-Fe(1)-N(2)	77.9(1)	77.90(8)	0.00

Table S2. Angles between equatorial planes and opposite faces in *t*-**1** and *m*-**1** (with their difference in %) at 293 K for *t*-**1** and 295 K for *m*-**1**

	Angles (°) in		
	t-**1**	*m*-**1**	Δ (%)
Planes			
O1 O2 N2 N3 O1 N2 N1 N4	84.79(8)	84.84(6)	0.1
O1 N2 N1 N4 O2 N3 N1 N4	88.39(8)	88.21(5)	0.2
O2 N3 N1 N4 O1 O2 N2 N3	86.13(8)	88.13(6)	2.3
Faces			
O1 O2 N4 N2 N3 N1	16.9(2)	16.9(1)	0.00
O1 O2 N1 N2 N3 N4	19.0(2)	13.4(1)	-29.5
O1 N3 N4 N2 O2 N1	7.0(2)	8.84(6)	26.3
O1 N3 N1 N2 O2 N4	20.5(2)	18.8(1)	-8.3

Table S3. Selected torsion angles in *t*-**1** and *m*-**1** and their comparison at at 293 K for *t*-**1**, 295 K for *m*-**1** and 180 K

Atoms	*t*-**1**, 295 K	*m*-**1**, *295 K*	*t*-**1**, 180 K	*m*-**1**, *180 K*	Δ% t-m/295	Δ % t-m/180	Δ % Tri	Δ % mono
C8-N1-C7-C6	-177.3(4)	*-177.2*(2)	-178.7(4)	*-176.8*(2)	-0.1	-1.1	*-0.8*	0.2
C7-N1-C8-C9	-159.5(4)	*-167.3*(2)	-144.6(4)	*-167.2*(2)	4.9	15.6	*9.3*	0.1
C10-N2-C9-C8	-75.4(4)	*-71.2*(3)	-89.3(5)	*-71.0*(2)	-5.6	-20.5	*-18.4*	0.3
C9-N2-C10-C11	160.3(3)	*162.9*(2)	85.5(5)	*163.6*(2)	1.6	91.3	*46.7*	-0.4
C12-N3-C11-C10	165.5(3)	*157.2*(2)	96.9(4)	*157.6*(2)	-5.0	62.6	*41.5*	-0.3
C11-N3-C12-C13	-71.3(4)	*-69.3*(3)	-77.1(5)	*-69.0*(2)	-2.8	-10.5	*-8.1*	0.4
C14-N4-C13-C12	-179.6(3)	*176.1*(2)	-160.0(4)	*173.9*(2)	**-198.1**	**-208.7**	*10.9*	1.2
C13-N4-C14-C15	-176.8(3)	*-178.4*(2)	177.6(4)	*-178.5*(2)	0.9	**-200.5**	*200.5*	-0.1
N1-C8-C9-N2	-44.3(3)	*-39.3*(3)	-43.8(5)	*-38.8*(2)	-11.3	-11.4	*1.1*	1.3
N2-C10-C11-N3	-55.6(4)	*-53.8*(3)	41.0(5)	*-54.6*(2)	-3.2	**-233.2**	*173.7*	-1.5
N3-C12-C13-N4	-32.6(4)	*-40.3*(3)	-43.0(5)	*-40.1*(2)	**23.6**	-6.7	*-31.9*	0.5

Table S4. List of short contacts (< sum of the van der Waals radii) in *t*-**1** and *m*-**1** at 293 K for *t*-**1** and 295 K for *m*-**1**

Contacts between		Atom 1	Atom 2	Symmetry operation to be applied on atom 2	Length
[Ni] moieties	*t*-**1**	S4	S8	x,-1+y,z	3.459(1)
	m-**1**	S6	S3	2-x,2-y,1-z	3.576(1)
		S2	S2	2-x,1-y,1-z	3.504(1)
		S4	S5	2-x,-1/2+y,1/2-z	3.513(1)
[Ni] and [Fe] moieties	*t*-**1**	C14	S3	-1+x,1+y,z	3.424(4)
		H3N	S7	x,y,z	2.89
		H112	S7	x,y,z	2.99
		H81	S2	x,y,z	2.99
		S7	H101	-x,-y,2-z	2.97
		S10	H111	-x,1-y,2-z	2.99
		S5	H121	x,-1+y,z	2.84
		S5	H2N	1+x,-1+y,z	2.60
	m-**1**	S7	H2N	x,y,z	2.68
		S6	H8A	x,1+y,z	2.80
		S1	H10A	x,1+y,z	2.99
		S10	H3N	x,1/2-y,1/2+z	2.55
		S10	C6	x,1/2-y,1/2+z	3.454(3)
		S5	H12B	2-x,1/2+y,1/2-z	2.84
[Fe] moieties	*t*-**1**	C14	C16	-x,1-y,1-z	3.306(6)
	m-**1**	C5	C7	1-x,-y,1-z	3.385(4)

[a] [Fe] and [Ni] stand for $[Fe(sal_2\text{-trien})]^+$ and $[Ni(dmit)_2]^-$

Table S5. List of C-C contacts (< 3.6 Å) in *t*-**1** and *m*-**1** at 293 K for *t*-**1** and 295 K for *m*-**1**

Compound	Number of contacts with the [Ni] and [Fe] moieties	Atom 1	Atom 2	Symmetry operation to be applied on atom 2	Length
t-**1**	17 with 4 [Fe][a] 2 with 1 [Ni][a]	C1	C4	1-x,-y,1-z	3.527(6)
		C6	C3	1-x,-y,1-z	3.531(6)
		C2	C5	1-x,-y,1-z	3.532(7)
		C3	C9	1+x,y,z	3.550(7)
		C16	C14	-x,1-y,1-z	3.306(6)
		C14	C17	-x,1-y,1-z	3.567(6)
		C15	C16	-x,1-y,1-z	3.571(6)
		C15	C15	-x,1-y,1-z	3.581(5)
		C14	C15	-x,1-y,1-z	3.593(5)
		C7	C21 (Ni)	x,y,z	3.529(5)
		C12	C25 (Ni)	x,y,z	3.584(6)
m-**1**	4 with 1 [Fe] 2 with 1 [Ni]	C4	C8	1-x,-y,1-z	3.596(5)
		C5	C7	1-x,-y,1-z	3.385(4)
		C16	C25 (Ni)	x,y,z	3.506(4)
		C16	C24 (Ni)	x,y,z	3.482(4)

[a] [Fe] and [Ni] stand for $[Fe(sal_2\text{-trien})]^+$ and $[Ni(dmit)_2]^-$