Auxiliary alkyl chain modulated spin crossover behaviour in $[Fe(H_2Bpz_2)_2(C_n\text{-bipy})]$ complexes

Yunnan Guo[a,b], Aurelian Rotaru[c], Helge Müller-Bunz[d], Grace G. Morgan[d], Shishen Zhang[a], Shufang Xue*[,a,b] and Yann Garcia*[,b]

Table S1 Selected bond lengths (Å), angles (°) and structural parameters for **4** and **5**

4			**5**		
	100	293		100	130
Fe1-N2	2.0146(13)	2.1952(18)	Fe1-N1	1.998(2)	2.1432(13)
Fe1-N4	1.9926(13)	2.1374(17)	Fe1-N3	2.020(2)	2.1976(13)
Fe1-N6	2.0152(13)	2.2067(18)	Fe1-N5	2.024(2)	2.1856(13)
Fe1-N8	1.9985(14)	2.1391(17)	Fe1-N7	1.998(2)	2.1443(12)
Fe1-N9	1.9746(13)	2.2293(16)	Fe1-N9	1.977(2)	2.2220(12)
Fe1-N10	1.9705(13)	2.2260(16)	Fe1-N10	1.982(2)	2.2439(12)
$Fe\text{-}N_{av(pz)}$	2.0052(13)	2.1696(17)	$Fe\text{-}N_{av(pz)}$	2.010(2)	2.1678(12)
$Fe\text{-}N_{av(bipy)}$	1.9726(13)	2.2277(16)	$Fe\text{-}N_{av(bipy)}$	1.9795(2)	2.2330(12)
N2-Fe1-N4	88.82(5)	87.56(7)	N1-Fe1-N3	88.53(10)	86.45(5)
N2-Fe1-N6	175.90(5)	177.95(7)	N1-Fe1-N5	88.35(10)	90.09(5)
N2-Fe1-N8	88.82(5)	92.68(7)	N1-Fe1-N7	88.19(10)	96.66(5)
N2-Fe1-N9	95.17(5)	94.04(6)	N1-Fe1-N9	95.94(10)	97.98(5)
N2-Fe1-N10	86.25(5)	84.87(6)	N1-Fe1-N10	176.12(10)	168.73(5)
N4-Fe1-N6	88.05(5)	90.81(7)	N3-Fe1-N5	176.07(10)	176.41(5)
N4-Fe1-N8	88.46(5)	97.63(7)	N3-Fe1-N7	87.85(10)	90.80(5)
N4-Fe1-N9	94.99(5)	94.72(7)	N3-Fe1-N9	96.45(10)	96.86(4)
N4-Fe1-N10	173.63(5)	164.73(6)	N3-Fe1-N10	89.01(10)	88.10(4)
N6-Fe1-N8	88.44(5)	86.29(7)	N5-Fe1-N7	89.66(10)	88.65(5)
N6-Fe1-N9	87.75(5)	87.34(6)	N5-Fe1-N9	86.26(10)	84.56(5)
N6-Fe1-N10	97.06(5)	97.00(6)	N5-Fe1-N10	94.23(10)	95.47(5)
N8-Fe1-N9	174.77(5)	166.17(6)	N7-Fe1-N9	174.09(10)	163.85(5)
N8-Fe1-N10	95.46(5)	95.96(6)	N7-Fe1-N10	94.72(10)	93.27(5)
N9-Fe1-N10	81.46(5)	72.66(6)	N9-Fe1-N10	81.35(10)	72.88(4)
CShMs[a]	7.452	7.944	CShMs[a]	7.973	8.843
Σ[b]	44.63	64.12	Σ[b]	42.14	60.49

[a] CShMs: continuous shape measure values. [b] Σ is the sum of the deviation from 90° of the 12 *cis* angles of the FeN_6 octahedron.

Table S2. Supramolecular interaction involving C-H···O, π···π stacking interactions as well as C-H···π interactions for **4** and **5**

Type	Complex	D-H···A (Å)	H···A(Å)	D···A (Å)	D-H···A(◦)	Symmetry code
C-H···O	**4**	C2-H2···O2	2.6688(12)	3.5305(2)	151.02(10)	*x*, -*y*, -0.5+*z*
		C33-H33A···O3	2.5532(26)	3.3023(15)	146.78(92)	-*x*, *y*, 0.5-*z*
	5	C8-H8···O1	2.6967(22)	3.5762(4)	157.99(20)	*x*, 1-*y*, 0.5+*z*
		C33-H33A···O3	2.5532(26)	3.3561(4)	140.34(20)	1-*x*, 1-*y*, 2-*z*
π···π stacking (Type A)		Centre···Centre (Å)				
	4	3.347				
	5	3.330				
C-H···π (Type B)		C-H···Centre (Å)				
	4	3.348				
	5	3.338				

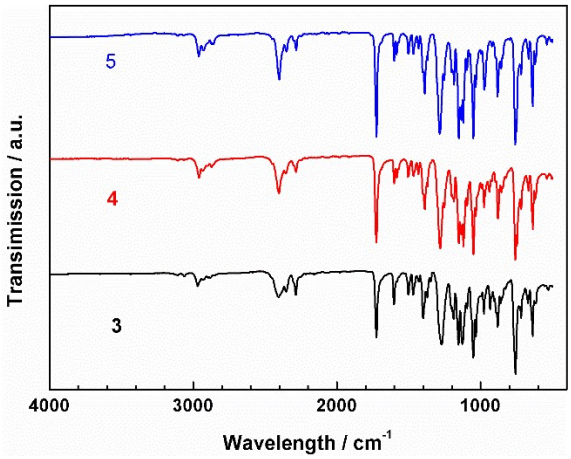

Fig. S1 IR spectra of powdered samples **3**-**5**.

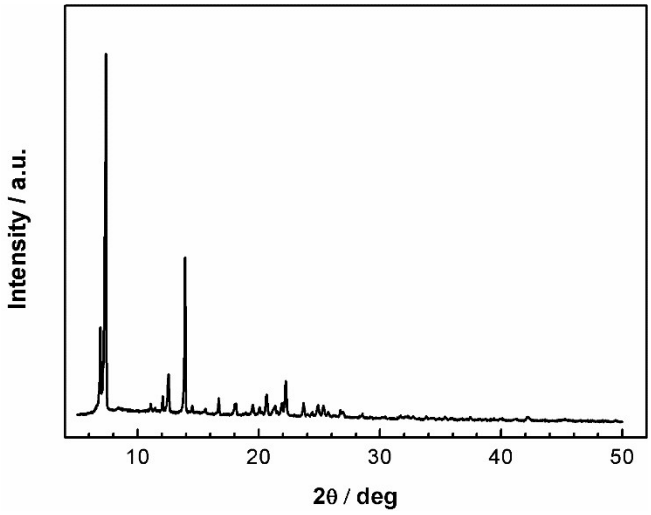

Fig. S2 X-ray powder diffraction patterns at 298 K for **3**.

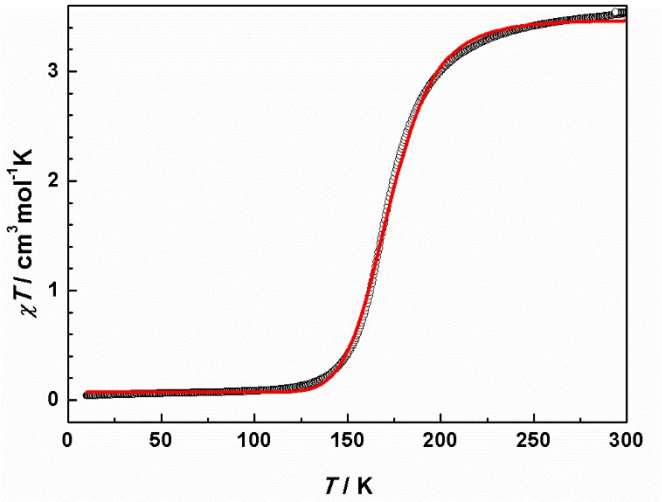

Fig. S3 Temperature-dependent $\chi_M T$ plots for **4**. The red solid curve corresponds to data fitting using the ideal solution model.[1]

Reference :

[1] O. Kahn. Molecular Magnetism, Wiley-VCH, New York, 1993.