

# Spin-Crossover Iron(II) Complexes With a Terpyridine Embrace Packing Motif Show Remarkably Consistent Cooperative Spin-Transitions

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## Electronic Supplementary Information

**Table S1** Selected bond lengths and angles for the high-spin tetragonal phases of  $[\text{Fe}(\text{L}^3)_2][\text{BF}_4]_2$  and  $[\text{Fe}(\text{L}^4)_2][\text{BF}_4]_2$ .

**Table S2** Selected bond lengths and angles for the low-spin monoclinic phase of  $[\text{Fe}(\text{L}^3)_2][\text{BF}_4]_2$  at 202 K.

**Figure S1** View of the complex dication in the monoclinic phase of  $[\text{Fe}(\text{L}^3)_2][\text{BF}_4]_2$  at 202 K.

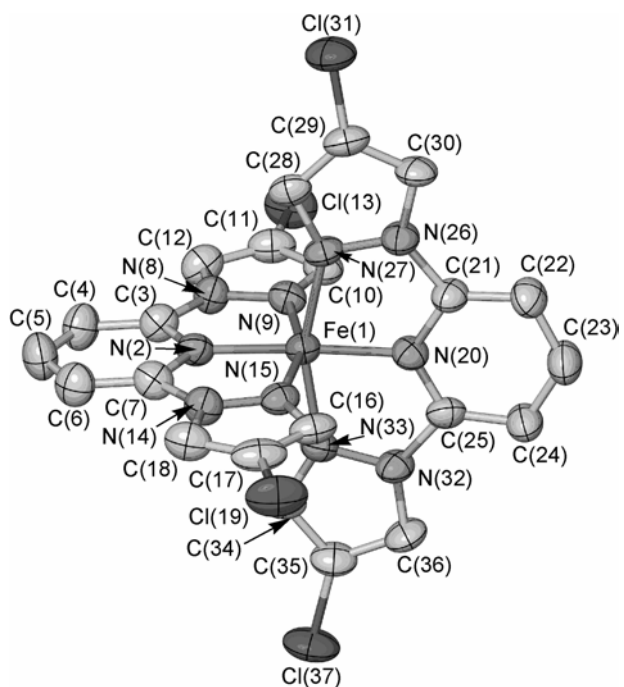
**Figure S2** View of the complex dication in the tetragonal phase of  $[\text{Fe}(\text{L}^4)_2][\text{BF}_4]_2$  at 300 K.

**Table S1** Selected bond lengths and angles (Å, °) for the high-spin tetragonal phases of  $[\text{Fe}(\text{L}^3)_2][\text{BF}_4]_2$  and  $[\text{Fe}(\text{L}^4)_2][\text{BF}_4]_2$ . Symmetry code (ii)  $-1+y, 1-x, 2-z$  (see Figs. 2 and S2).

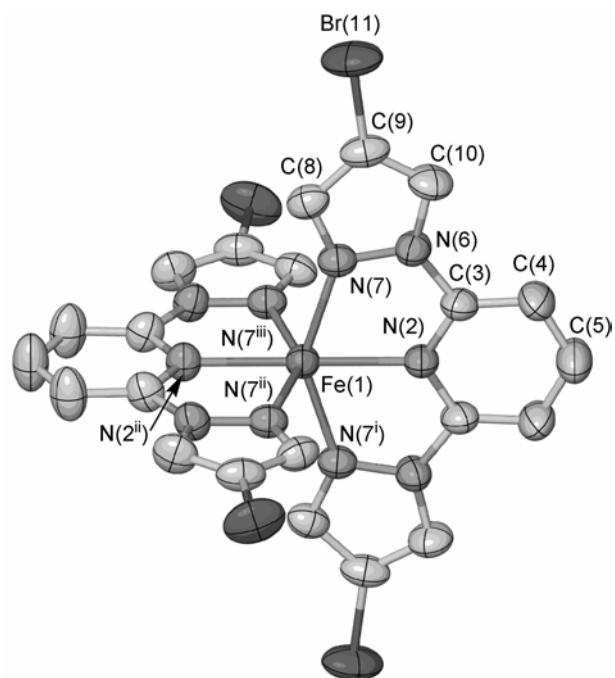
	$[\text{Fe}(\text{L}^3)_2][\text{BF}_4]_2$		$[\text{Fe}(\text{L}^4)_2][\text{BF}_4]_2$
	300 K	220 K	300 K
Fe(1)–N(2)	2.135(3)	2.143(5)	2.125(4)
Fe(1)–N(7)	2.188(2)	2.180(4)	2.188(3)
N(2)–Fe(1)–N(2 <sup>ii</sup> )	180	180	180
N(2)–Fe(1)–N(7)	72.97(6)	73.23(10)	73.46(8)
N(2)–Fe(1)–N(7 <sup>ii</sup> )	107.03(6)	106.77(10)	106.54(8)
N(7)–Fe(1)–N(7 <sup>ii</sup> )	94.92(3)	94.77(5)	94.65(5)

**Table S2** Selected bond lengths and angles (Å, °) for the low-spin monoclinic phase of  $[\text{Fe}(\text{L}^3)_2][\text{BF}_4]_2$  at 202 K.

Fe(1)–N(2)	1.898(5)
Fe(1)–N(9)	1.974(5)
Fe(1)–N(15)	1.955(6)
Fe(1)–N(20)	1.890(5)
Fe(1)–N(27)	1.985(5)
Fe(1)–N(33)	1.963(6)
N(2)–Fe(1)–N(9)	79.8(2)
N(2)–Fe(1)–N(15)	80.1(2)
N(2)–Fe(1)–N(20)	176.9(3)
N(2)–Fe(1)–N(27)	102.5(3)
N(2)–Fe(1)–N(33)	96.8(3)
N(9)–Fe(1)–N(15)	160.0(2)
N(9)–Fe(1)–N(20)	101.4(2)
N(9)–Fe(1)–N(27)	92.7(2)
N(9)–Fe(1)–N(33)	91.6(2)
N(15)–Fe(1)–N(20)	98.7(2)
N(15)–Fe(1)–N(27)	91.3(2)
N(15)–Fe(1)–N(33)	91.0(2)
N(20)–Fe(1)–N(27)	80.3(2)
N(20)–Fe(1)–N(33)	80.4(2)
N(27)–Fe(1)–N(33)	160.7(2)



**Fig S1** View of the complex dication in the monoclinic phase of  $[\text{Fe}(\text{L}^3)_2][\text{BF}_4]_2$  at 202 K. All H atoms have been removed for clarity, and thermal ellipsoids are at the 50% probability level.



**Fig S2** View of the complex dication in the tetragonal phase of  $[\text{Fe}(\text{L}^4)_2][\text{BF}_4]_2$  at 300 K. All H atoms have been removed for clarity, and thermal ellipsoids are at the 50% probability level. Symmetry codes: (i)  $-x, 2-y, z$ ; (ii)  $-1+y, 1-x, 2-z$ ; (iii)  $1-y, 1+x, 2-z$ .