Anion-Solvent Dependence of Bistability in a Family of Meridional N-Donor Ligand Containing Iron(II) Spin Crossover Complexes.

*Ben A Leita,[a] Suzanne M. Neville,[a] Gregory J. Halder,[b] Boujemaa Moubaraki,[a] Cameron J. Kepert,[b] Jean-François Létard[c] and Keith S. Murray,[*a]*

[a] School of Chemistry, Building 23, Monash University, Clayton, Victoria 3800, Australia.

[b] School of Chemistry, University of Sydney, NSW 2006, Australia.

[c]ICMCB, CNRS, Université Bordeaux 1**,** 87 avenue du Dr. A. Schweitzer**,** 33608 Pessac cedex France

***** To whom correspondence should be addressed. E-mail: keith.murray@sci.monash.edu.au. Tel: +61-3-99054512. Fax: +61-3-99054597.

S1: Single crystal X-ray diffraction analysis

Table S2. Hydrogen-bonding interactions in 1·MeOH

Table S3. Intermolecular interactions in 1·MeOH

S4: Database of $T_{½}$ versus T(LIESST)

S1: <u>Single crystal X-ray diffraction analysis</u>

Special refinement details. The thermal parameters of equivalent disordered components were constrained to be the same. Excluding the fully LS structure (25s), the methanol molecule is disordered over two sites (A and B), both sharing the C30 methyl position. The A and B components refined to give occupancy ratios of 58:42 (25q), 49:51 (123 K) and 46:54 (293 K). The bond length of the B orientation of the methanol molecule was constrained to a length of 1.41(2) Å. The F4 atom of the 123 K structure and the F2 and F4 atoms of the 293 K structure are disordered over two sites (A and B), with refined occupancy ratios of 47:53 (123 K) and 43:57 (293 K).

Table S2. Hydrogen-bonding interactions in 1·MeOH

Hydrogen Bonds(Å)	25s	25q	123	293
O30…F8	2.837(3)	2.795(4)	-	-
O30A…F8	-	-	2.825(6)	3.018(18)
O30B…F3	-	2.903(6)	2.912(6)	3.108(14)
O30B…F4A	-	-	3.315(8)	-
O30B…F4B	-	-	3.005(7)	2.809(19)

Table S3. Intermolecular interactions in 1·MeOH

Interactions (Å)	25s	25q	123	293
N2…C(H)π	3.583(3)	3.240(6)	3.262(6)	3.240(10)
N7…C(H)π	3.122(3)	3.052(5)	3.085(8)	3.118(14)

S4: Database of $T_{½}$ versus T(LIESST)

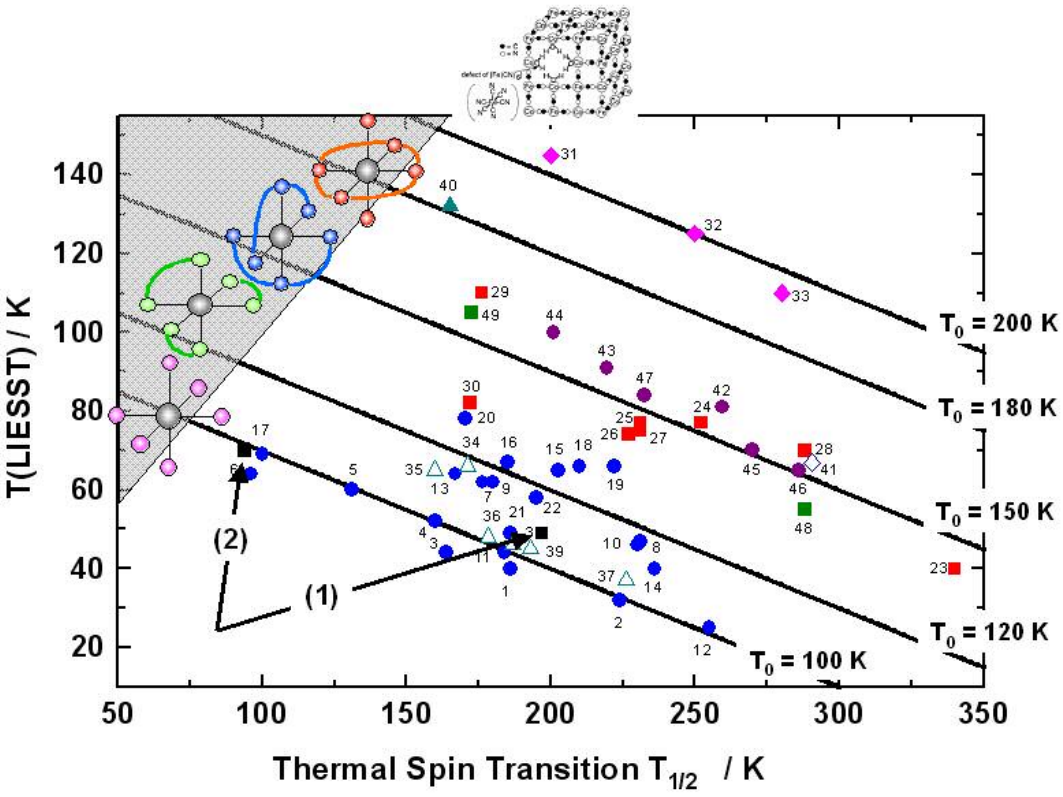

Figure S4 Variation of T(LIESST) versus $T_{½}$ for spin crossover compounds by Létard *et al*. The black squares show where $[Fe(picpzpz)_2](BF_4)_2$·MeOH, **1·MeOH**, fits, (**1**) $T(LIESST)_1$ = 49 K and (**2**) $T(LIESST)_2$ = 70 K. The region in grey is meaningless as the T(LIESST) temperature has to be inferior or at least equal to $T_{½}$. Identification for the compounds 1 – 49 can be found in references 12 and 19 in text.