**Heteroleptic Fe(II) Spin-Crossover Complexes with a N4S2 Coordination**

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**Introduction**

Spin-crossover (SCO) compounds supported by first-row transition metals have attracted significant interest due to their magnetic bistability which is coupled with dramatic changes in structural and optical properties. Such multifarious switching can take place tersely and hysteretically and is induced by changes in temperature, pressure or through photoexcitation. Consequently, materials based on such SCO complexes constitute promising candidates for applications in memory, sensing and display devices. While ferrous compounds with a coordination sphere consisting of six nitrogen-donor atoms account for most of the known SCO compounds we and others have recently demonstrated the occurrence of SCO behavior for iron(II)-based complexes incorporating a N4S2 coordination.1,2 Specifically, we have investigated a series of complexes supported by S,S’-bis(2-pyridilmethyl)-1,2-thioethane (bpte) in combinations with 2,2’-biimidazole (bim) and 1,1’-(α,α’-*o*-xylyl)-2,2’-biimidazole (xbim), that is, [Fe(bpte)(bim)]X2 and [Fe(bpte)(xbim)]X2 where X = ClO4-, BF4-, OTf-.

**Experimental**

Samples of heteroleptic Fe(II) ions supported by bpte, xbim, and bim ligands were investigated using the high-field Mössbauer spectrometer available in the EMR facility.

**Results and Discussion**

The magnetic properties including the temperature-dependent 57Fe Mössbauer spectra of the complexes examined in this work indicate that the bpte ligand provides a slightly stronger ligand field as compared to the similar tetradentate ligand, tpma, which was used by us previously to obtain heteroleptic SCO complexes [Fe(tpma)(bim)](ClO4)2·0.5H2O and [Fe(tpma)(xbim)](ClO4)2, with T1/2 of 190 and 200 K, respectively. Thus, while the typical coordination environment of Fe(II) SCO complexes contains six N-donor sites, our results demonstrate that the {N4S2} coordination appears to be a promising platform for the design of new SCO materials.

**Fig.1** Zero-field 57Fe Mössbauer spectra recorded at 4.2 K and 298 K for [Fe(bpte)(bim](ClO4)2 (a) and [Fe(bpte)(bim)](BF4)2 (b). The solid gray lines overlaid on the 298 K spectra are simulations obtained from the sum of the low-spin component (red trace) and high-spin components (blue traces).

**Conclusions**

This study expands the range of known coordination environments that can lead to a spin-crossover behavior for iron(II) ions.

**Acknowledgements**

The 57Fe Mössbauer spectra were recorded at the NHMFL, which is funded by the NSF through the Cooperative Agreement No. DMR–0654118, the State of Florida and the DOE. The Mössbauer instrument was funded by the UCGP-5064 grant (to A. Ozarowski). This work was also supported by the US NSF award CHE-1464955 to MS.

**References**

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