MS13-2-21 A structural study by single-crystal X-ray diffraction of iron(III) [Fe(5-X-Salmeen)$_2$]BF$_4$ #MS13-2-21

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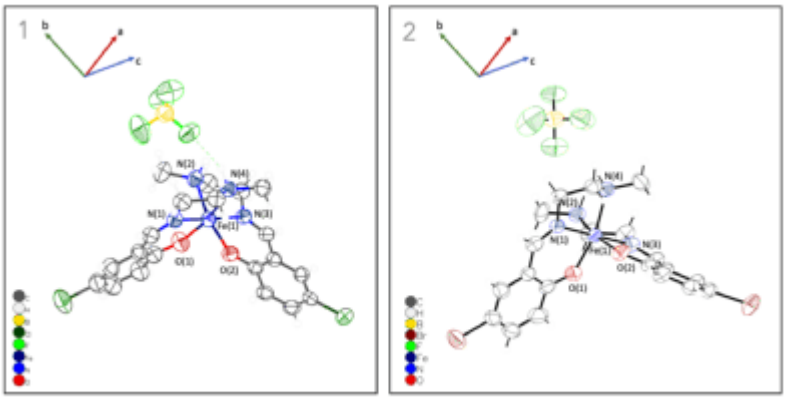
Abstract
Spin-crossover (SCO) compounds are switchable between two electronic spin states, Low spin (LS) and High spin (HS). In general, the switching process in solid-state systems is controlled by cooperative intermolecular interactions.[1]
The correlation of structure with physical properties is crucial for identifying these interactions and ultimately understanding the complex processes controlling the SCO phenomenon.
Against this background, we carried out the synthesis and characterization of two coordination compounds candidates for SCO phenomenon, [Fe(5-Cl-Salmeen)$_2$]BF$_4$ and [Fe(5-Br-Salmeen)$_2$]BF$_4$, where substituted Salmeen result from the Schiff-base condensation of substituted salicylaldehyde with N-methylethylenediamine.
The structural study was performed by single-crystal X-ray diffraction for five temperatures between 170 to 293K, revealing that coordination compound cations 1-2 (Fig. 1) are isostructural with N4O2 donor atom set from tridentate ligands forming a distorted octahedron around the Fe(III) ion.
Both complexes crystallize in the monoclinic spacial group P21/n, containing two molecules of the cationic Fe(III) complex (Z'=2), where fragment 1 and fragment 2 have a different octahedral distortion, fragment 1 exhibits large values, consistent with the HS at 170 - 293K (Fig.2). While fragment 2 displays small values at 170K and high values at 293K, consistent with LS and HS states, respectively.
For both cases, the studies of the intermolecular interaction reveal differences in the percent of H-X, X-X, and X-F interactions between fragments 1 and 2.
Finally, the complex has been compared with the reported isostructural complex [Fe(5-Br-Salmeen)$_2$]ClO$_4$.[2]

References
[1] K. Ridier, G. Molnár, L. Salmon, W. Nicolazzi y A. Bousseksou. "Hysteresis, nucleation and growth phenomena in spin-crossover solids". Solid State Sciences 74 (2017), A1-A22. Doi: 10.1016/j.solidstatesciences.2017.10.014.[2] M. Wang, G Lee, Y. Wang, T. Dong y H. Wei. "Structure, magnetic properties, Mössbauer and catalase-like activity of spin crossover iron(III) complexes with salicylaldimine ligands". Journal of the Chinese Chemical Society 49(5) (2002), 825-832. Doi: 10.1002/jccs.200200118.

ORTEP diagram for fragment 1 of complexes 1 and 2.



Multi-scale representation of structural changes