Proposal 16-01-699
Structural characterization of cyanide-bridged metal-organic complexes
Time allocated: 6 shifts

Although, a great effort in the synthesis have been devoted to these compounds due to their potential applications (catalysis, room temperature magnets, photomagnetism and magneto-optics), one of the main problems, we have to face is the tiny size of the crystals obtained (from 60 to 100 microns in all the three directions). So, synchrotron radiation was the key factor that allowed us to obtain a quality data set for these complexes. In this proposal, we have tried to solve the crystal structure of a family of cyano-bridged compounds of general formula $[M^{III}L2(CN)_2][Fe^{III}L1(CN)_4]$, where L1 and L2 are different ligands.

Using the PX beamline of BM16 we were able to collect, solve and refine the following complexes:

1. $[Mn^{III}(3MeOsalen)][Fe^{III}(bpym)(CN)_4]$; where 3MeOsalen = N,N'-ethylenebis(3-methoxysalicylideneiminate) and bpym = 2,2'-bipyrimidine.
2. $[Mn^{III}(3MeOsalen)][Fe^{III}(dmbipy)(CN)_4]$, where dmbipy = 4,4'-dimethyl-2,2'-bipyridine.
3. $[Mn^{III}(salpn)][Fe^{III}(bpym)(CN)_4]$ where salpn = *N*,*N*'-bis(salicylidene)-1,3-diaminopropane.
4. $K_3Na[WO_2(CN)_4][Cu(tren)]$ where tren = tris(2-aminoethyl)amine. This latter complex is not part of the family under study but a prospect into using the $[WO_2(CN)_4]$ anion as a precursor.

We have some problems in the resolution of compound 4. Probably the selection of a better crystal and data collection with high redundancy will allow us, in a next run to obtain better results. Also, those crystals which did not diffract by various problems, small size, degradation by desolvation, crystallinity loss... will be appointed for a next proposal.

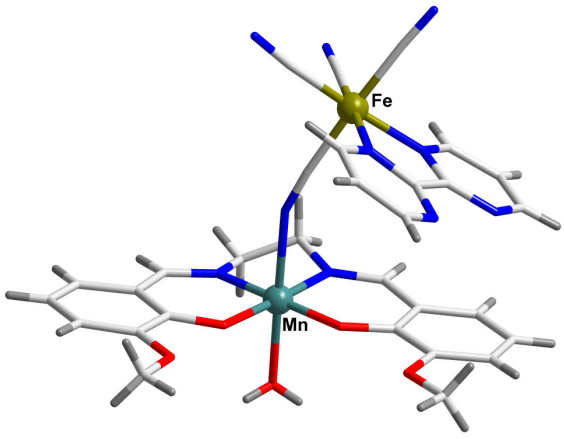

Figure 2. Schematic view of the precursor $[FeL1(CN)_4]^-$ with the cation $[MnL2(CN)_2]^+$, with L1 = bpym and L2 = 3MeOsalen, also one of the CN groups that surround the manganese cation has been interchanged by a water molecule.

Redaction and publication of the crystal structure of these compounds are now in progress.