

# Poster Presentations

## [MS10-P17] Structural Study of Two Ferrocenyl Derivatives with C≡N Groups: FcCH<sub>2</sub>CN and FcC(O)CN.

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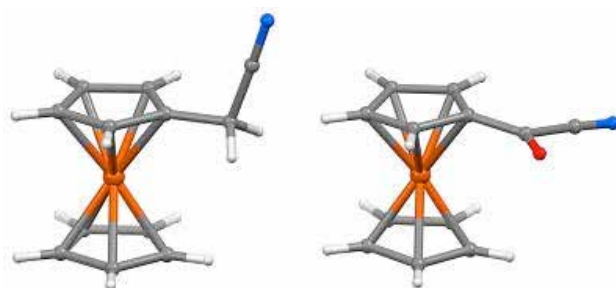
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The synthesis and study of ferrocene derivatives is an important and active research field [1], due to the fact that the ferrocene unit has an excellent air, thermal and photochemical stability, and it exhibits unique and valuable redox properties [2]. As a consequence, functionalised ferrocenes are exceptionally valuable scaffolds for the construction of functional molecules with potential applications in various areas of research including catalysis, materials science, molecular recognition and biomedical chemistry.

Among the large number of ferrocenes that have been described, derivatives with cyano groups are not very common. Following our previous work in the synthesis and study of ferrocene containing compounds [3-5], we present here the structural characterisation of two cyano ferrocene derivatives, namely cyanomethylferrocene, FcCH<sub>2</sub>CN; and 1- cyanocarbonylferrocene, FcC(O)CN. The carbonyl derivative has been obtained from FcCH<sub>2</sub>CN, by an innovative and environmentally friendly solvent-free silica-gel mediated mechanochemical reaction, and possesses interesting redox properties. Indeed, cyanocarbonylferrocene FcC(O)CN exhibits the highest Fe<sup>II</sup>/Fe<sup>III</sup>  $E_{1/2}$  oxidation potential reported for monosubstituted ferrocenes.

**Figure 1.** Molecular structures of the two cyano-substituted ferrocenes FcCH<sub>2</sub>CN (left) and FcC(O)CN (right).



In both cases the asymmetric unit comprises a molecule of the compound. The structural types of both cyano-substituted ferrocenes also show similar cell parameters, *Z*, and almost identical density values. The substituent attached to the ferrocene moiety, however, adopts a very different position in both cases (see figure 1), and this fact gives rise to quite dissimilar molecular arrangements for the two compounds. The supramolecular packing is achieved, in both cases, through weak intermolecular forces. A topological analysis of the two solid state structures has also been performed.

[1] *Ferrocenes: Ligands, Materials and Biomolecules*, ed. P. Stępnicka, Wiley, UK, 2008.

[2] *Inorganic Electrochemistry*; 2nd edn; eds. P. Zanello, F. Fabrizi de Biani, C. Nervi; Royal Society of Chemistry: Cambridge, 2012, pp. 173-247.

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**Keywords:** cyanoferrocenes; weak intermolecular forces; green chemistry