Experimental Report

Proposal: **5-12-303** **Council:** 10/2012

Title: Peculiar metal complex conformations - are the hydrogens really so close?

This proposal is a new proposal

Researh Area: Chemistry

Main proposer: **LUSI Matteo**

Experimental Team: LUSI Matteo
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Samples: C10 H8 N2 Br2 Zn1

Instrument	Req. Days	All. Days	From	To
D19	6	4	14/03/2013	18/03/2013

Abstract:

It has been observed that in some crystal structures the distance between hydrogen atoms can be shorter than the sum of their van der Waals radii. This is particularly frequent in metal complexes of 2,2'- and 4,4'-bipyridine in which the ligand is forced in a flat conformation. By collecting accurate neutron diffraction data for archetypes of these spices the project herein presented aims to understand if this is really the case and how it is possible. The results will help redetermining precise value of the hydrogen radii. Benefits are foreseen for the design of this class of chemicals, which are of particular interest as pharmaceuticals as well as in material science.

Due to the beam time assigned the experiment, originally proposed for the determination of a number of structures with general formula [MX_2(2,2′-bipy)] (with M = transition metal and X + any halogen), focused on the determination of [CuBr (2,2′-bipy)$_2$]Br (**1**). The structures determined at 100 K confirms that **1** is distorted from the idealised geometry as calculated by DFT. The same behaviour is observed in all the other 3 cases reported on similar structure types solved by Neutron radiation.

In order to further investigate the causes of distorted geometry the Neutron determined structure was used as a model for DFT analysis. The preliminary results indicate that the interaction of the H atoms in position 6 and 6′ have is the main responsible for the observed geometry. Those preliminary results have been presented in an oral symposium at the 28th European Crystallography Meeting in Warwick.

The nature of such interaction is currently investigated computationally and by Charge Density Analysis. Moreover, other crystals with similar structure are currently being collected at the BRAGG institute to verify the generality of such behaviour. A journal article will soon summarize the results.