Metal-Ligand and Metal-Metal Bonding Characterization from X-ray Diffraction

Nouzha Bouhmaida[1], B. Fraisse[2], A. Perez-Benítez[3], M.A. Méndez-Rojas[4], N.E. Ghermani[2,5], *[1]LSM, Université Cadi Ayyad, Faculté des Sciences Semlalia, Boulevard Moulay Abdallah, BP 2390, 40000 Marrakech, Morocco. [2]Ecole Centrale Paris, SPMS UMR CNRS 8580 1, Grande Voie des Vignes, 92295 Châtenay-Malabry, France. [3]Facultad de Ciencias Químicas, Benemérita Universidad Autónoma de Puebla, Puebla 72000, México. [4]Departamento de Química y Biología, Universidad de las Américas-Puebla, Ex-Hacienda Sta. Catarina Mártir, Cholula, 72820 Puebla, Pue., Mexico. [5]PPB UMR CNRS 8612, Faculté de Pharmacie 5, Rue Jean-Baptiste Clément, 92296 Châtenay-Malabry, France.* E-mail: nouzha@ucam.ac.ma

The metal complex of a non-steroidal anti-inflammatory drug (NSAID), di-μ-aspirinato-copper(II), crystallizes in its biochemical active form [1]. The electron density and electrostatic potential calculations are useful for the understanding of the metal-ligand bonding and its connection with the biochemical activity of such molecule. The compound also offers the opportunity to characterize the occurring copper-copper bond (Cu – Cu = 2.604 Å).

X-ray diffraction measurements were performed on a smart CCD diffractometer at 100 K with the MoKα radiation. up to sin θ/λ= 1.11 Å^{-1}. The compound crystallizes in the $P2_1/c$ group and reveals a one dimensional polymeric structure. The copper is in an irregular octahedral coordination corresponding to five oxygen atoms and one copper.

Electron density refinements are carried out using the Hansen-Coppens model [2]. The Cu-O, Cu-Cu electron density bonds are discussed according to the copper d-orbital populations. Electrostatic potential and active sites of the molecule are also shown.

[1] Garcia F., Méndez-Rojas M.A., González-Veraga E., Bernes S., Quiroz M.A., *Acta Cryst.*, 2003, **E59**, m1171-m1173. [2] Hansen N., Coppens P., *Acta Cryst*., 1978, **A34**, 909.

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