# Crystal structures of2-morpholino-5-nitrobenzaldehyde and 5-Nitro-2-(piperidino)benzaldehyde

*Frédérica Koblavi-Mansilla[1], Moussa KONE[1], Aka Joseph N\'GOUAN[1], Yapi Marcellin YAPO[1]*

*[1]Laboratoire De Cristallographie Et Physique Moléculaire UFR SSMT Université FHB, Abidjan, Ivory Coast*

*E-mail: fmkoblavi@hotmail.com*

The investigation of the atomic and molecular structure of therapeutic or toxic compounds is important because it helps to understand their mechanism of action. Nitroaromatics are reactional intermediate compounds in chemical synthesis well known for their toxicity. In order to have a best insight of their structures and then to undertake a study of their possible toxic activities, we report here the single-crystal X-ray determination of two nitrobenzene derivatives compounds:2-Morpholin-4-yl-5-nitro-benzaldehyde and 5-Nitro-2-piperidino-benzaldehyde

From the X-rays diffraction, the structure of both compounds has successfully been solved. The parameters of agreement R obtained are satisfying (4.50% and 5.30%).

The analysis and interpretation of the geometrical characteristics relating to bond distances compared to standard values indicate that carbon-oxygen bonds: [d(C10-O4) = 1.420(2)Å and d(C9-O4) = 1.422(2) Å] are characteristic of simple bond between carbon sp3 and oxygen sp2 [C(sp3)-O(sp2)]. On the other hand, the distance d(C7-O3) = 1.194(1)Å is slightly shorter than the standard value (1.210Å) indicates a double bond between carbon sp2 and oxygen sp1 [C(sp2) = O(sp1)]. Bonds distances nitrogen-oxygen: [d(O1-N1)=1.214(1)Å and d(O2-N1) =1.207(1)Å] indicate characteristic values of nitrogen-oxygen bonds in the nitro group (NO2). This assumption is confirmed by carbon- nitrogen bond distance: d(C1-N1)=1.457(1)Å which corresponds to simple bond between an aromatic carbon and nitrogen [Car-NO2]. For aromatic ring, bond angles present no particularity. Indeed, bond angles values are nearly equal to 120° which represents average value observed in aromatic ring.

The geometry and stacking in the crystals have been explained and that is essential to understand their behavior in synthesis.

We retain that, the substituents on a molecule influence the bond lengths and bond angles in the geometrical structure. Also the stability in these molecules is governed by hydrogen bonds.

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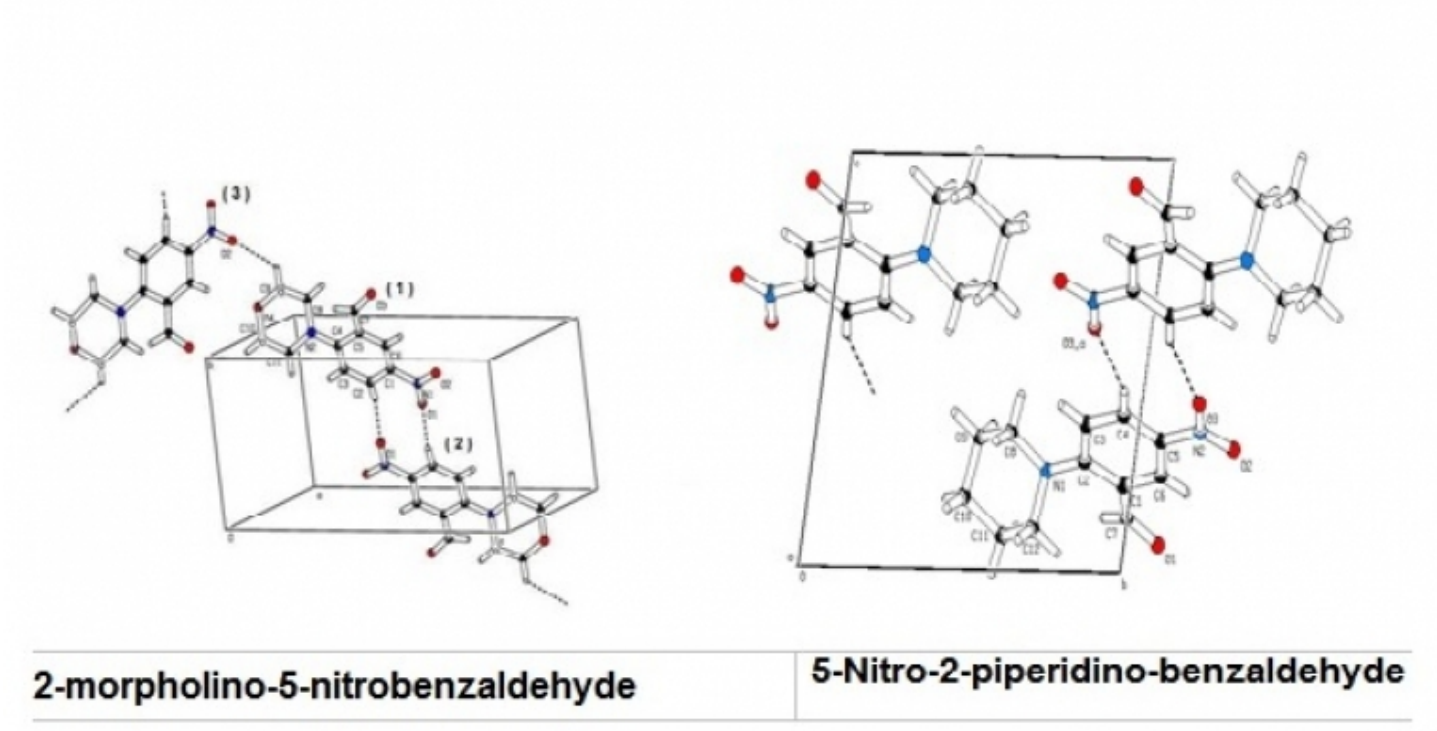


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