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THE CRYSTAL STRUCTURES OF N-(4-NITROBENZYLIDENE)-2-METHOXY-5-AMINOPYRIDINE

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Abstract: N-(4-Nitrobenzylidene)-2-methoxy-5-aminopyridine crystallizes in two crystalline forms: centrosymmetric (monoclinic $P2_1/n$), and non-centrosymmetric (monoclinic, $P2_1$). This study compares the molecular structures of the two crystalline forms.

INTRODUCTION

As part of our ongoing studies of the effects of the aromatic substitution on the optical or electro-optical properties of crystalline Schiff bases, we present this report on the centrosymmetric and non-centrosymmetric structure of the Schiff base of 4-nitrobenzaldehyde with 5-amino-2-methoxypyridine.

RESULTS AND DISCUSSION

The title compound crystallizes in two crystalline forms (i) centrosymmetric[1], monoclinic $P2_1/n$, a = 11.080(2) Å, b = 8.376(1) Å, c = 14.364(2) Å, β = 112.56(1)°, Z = 4, R = 0.0374 and (ii) non-centrosymmetric, monoclinic, $P2_1$,

a = 3.8566 Å, b = 19.542 Å, c = 8.066 Å, β = 89.37°, Z = 2 and R = 0.0489.

The centrosymmetric modification presents a planar form while the non-centrosymmetric, a non-planar form. The deviations from planarity among planes 1,2 and 3 (see Fig.1) for the two forms are as follows:

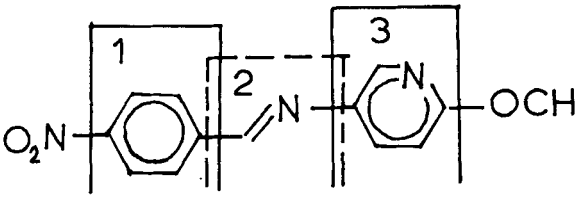


FIGURE 1. Deviations from planarity among planes 1,2 and 3 of the N-(4-Nitrobenzylidene)-2-methoxy-5-amino-pyridine molecule.

CENTRIC PLANAR FORM		ACENTRIC NON-PLANAR FORM
3.2°	between planes 1 and 2	4.8°
-22.7°	between planes 2 and 3	-31.8°
-19.6°	between planes 1 and 3	-35.7°

The bond lengths and bond angles of the centric planar form and of the acentric non-planar form are shown in Fig.2.

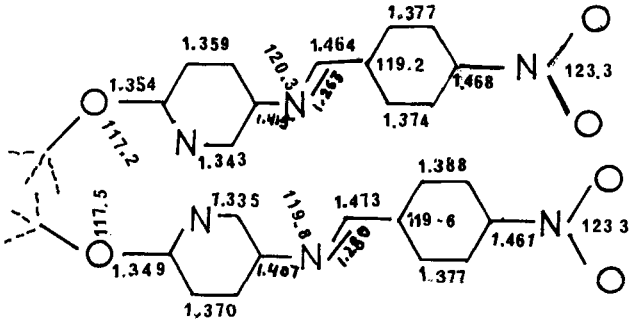
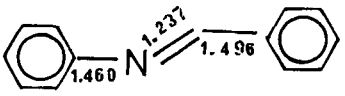


FIGURE 2. Bond lengths and bond angles of the centric planar form (upper) and of the acentric non-planar form (lower) of N-(4-Nitrobenzylidene)-2- methoxy-5--aminopyridine.

A comparison of the two structures results in the following observations:

1. The two structures have very similar bond distances and angles.
2. The OMe group is co-planar with the pyridine ring and facing the hetero N-atom.
3. The orientation of the above set of groups with respect to the rest of the molecule is opposite in the two structures.
4. The same trend in the differentation of the bridge bonds as compared to benzylideneaniline, indicating quinoid resonance structures and charge transfer between the elec-



tron donating and attracting groups.

5. Non-planarity of the molecule does not affect the internal charge transfer.
6. The non-centrosymmetric crystals have a high non-linear optical coefficient[2].

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2. to be published.