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# Michael addition of phenylacetonitrile to the acrylonitrile group leading to diphenylpentanedinitrile. Structural data and theoretical calculations

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Knoevenagel condensation of phenylacetonitrile with 4-diphenylaminophenylacetonitrile in the presence of piperidine was carried out to obtain a novel conjugated compound. In addition to the expected compound 2-(phenyl)-3-(4-diphenylaminophenyl)acrylonitrile (*I*), the 3-((4-diphenylamino)phenyl)-2,4-diphenylpentanedinitrile (*II*) was also obtained with a good yield. Compound *II* was obtained as a result of the Michael addition of phenylacetonitrile with 2-(phenyl)-3-(4-diphenylaminophenyl)acrylonitrile (*I*). Conversely, when the same reaction was performed in the presence of KOH as catalyst, only the $\alpha,\beta$-unsaturated nitrile (*I*) was afforded with a 92 % yield. The structures were confirmed with IR, EI-MS and NMR spectroscopy. Single crystals *I* and *II* were formed and their structures were determined by X-ray single-crystal diffraction analysis. Crystal *I* belongs to the monoclinic system with space group $P2_1/n$ having unit cell parameters of $a = 16.8589(5)$ Å, $b = 6.68223(17)$ Å, $c = 19.8289(7)$ Å, $\beta = 111.133(4)^\circ$ and $Z = 4$. Crystal *II* belongs to the same monoclinic system with space group $P2_1/c$, having unit cell parameters of $a = 10.8597(4)$ Å, $b = 24.7533(10)$ Å, $c = 9.7832(4)$ Å, $\beta = 91.297(3)^\circ$ and $Z = 4$. In addition to the structural data analysis, some theoretical calculations that reveal the nature of relevant structure–property relationships are also reported.


**Keywords:** phenylacetonitrile, $\alpha,\beta$-unsaturated nitrile, *N*-diphenylaminophenyl derivative, cyano-substituted compound, Michael addition, crystal structure

## Introduction

Unsaturated nitriles play a key role in several pathways proposed for the pre-biotic synthesis of biological molecules (Guillemin et al., 1998). Arylacrylonitriles are important synthons for the synthesis of several biologically active molecules used in the preparation of perfumes (Fraysse, 1980), flavonoid pigments (Fringuelli et al., 1994), sexual pheromones and vitamin A, etc. They are directly involved as plant growth regulators in increasing the soybean crop (Mori, 1976), and as inhibitors of prostaglandin synthetase (Peat et al., 1981; Michel et al., 1984). The traditional preparation of arylacrylonitriles involves the reaction of aromatic aldehydes with arylacetonitriles (Knoevenagel reaction, as well as Meyer and Frost reaction) (Knoevenagel, 1896; Frost, 1889). The compounds can be obtained under basic conditions in a polar solvent (NaOH, KOH, NaOEt, $K_2CO_3$ in MeOH, EtOH or THF) (D'sa et al., 1998; Guil-

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