

New carbazole substituted imines structure: synthesis and XRD analysis

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Imines represent an important class of molecules that are widely used (as intermediates) in the synthesis of a number of N-heterocyclic compounds [1]. These molecules are a product of reversible condensation of an amine and an aldehyde formed through the dynamic bond (a thermodynamically favored product).

General procedure for the synthesis of new carbazole substituted imines: 14.26 mmol of 3-amino-9-ethylcarbazole were dissolved in ethanol (30 ml) and added to 14.26 mmol Na₂CO₃ and 14.26 mmol aldehydes derivatives. The reaction mixture was then refluxed for 24 hours at 90°C. The solution was extracted with AcOEt with an aqueous phase. The organic phase was washed three times with water, dried with anhydrous magnesium sulphate, and evaporated under reduced pressure.

The X-ray diffraction (XRD) data for the imines samples were collected using a Bruker-Nonius KappaCCD single-crystal diffractometer (Mo K α radiation, $\lambda = 0.71073 \text{ \AA}$), installed at IC-CNR, Bari, Italy

The structures were solved by Direct Methods implemented in SIR2014 [2] and refined by SHELXL2014 [3] using a full-matrix least-squares method based on F². The non-hydrogen atoms were refined anisotropically. All the structures were characterized by non-negligible hydrogen bonds.

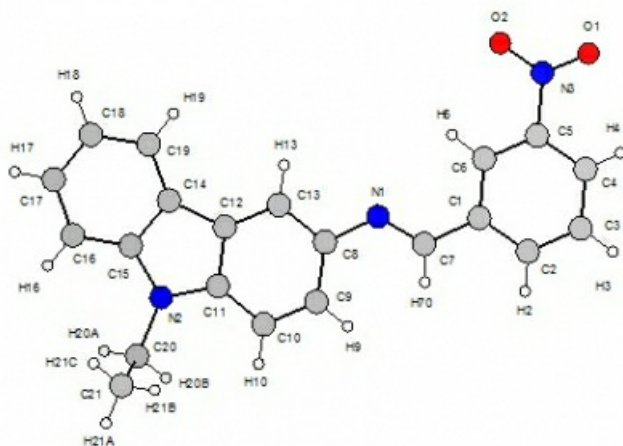
In Figure the molecular structure of one of the imine compounds [N-(5-nitrobenzylidene)-9-ethyl-9H-carbazol-3-amine (C₂₁H₁₇N₃O₂)] is shown.

The steps of imines synthesis and the main crystallographic results of the single crystal XRD study of the imines compounds will be described.

[1] Eicher, T., Hauptmann, S. & Speicher, A. (2012). The Chemistry of Heterocycles: Structures, Reactions, Synthesis, and Applications Third Edition. Wiley-VCH Verlag GmbH & Co. KGaA.

[2] Burla, M. C., Caliandro, R., Carrozzini, B., Cascarano, G.L., Cuocci, C., Giacovazzo, C., Mallamo, M., Mazzone A. & Polidori, G. (2015). J. Appl. Cryst. 48, 306-309.

[3] Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.



Keywords: [Imine](#), [synthesis](#), [single crystal XRD](#)