



Synthesis, Characterization, Structural Elucidation and Hirshfeld Surface Analysis of a Novel *1H*-Imidazole Derivative

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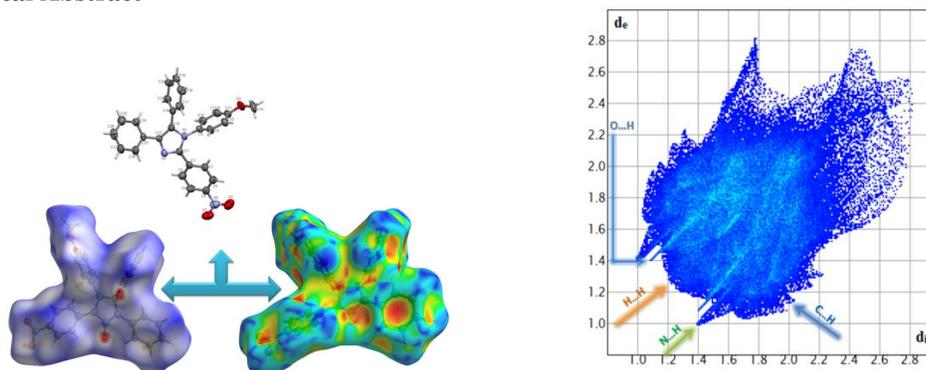
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ABSTRACT

A simple synthesis of 1-(4-methoxyphenyl)-2-(4-nitrophenyl)-4,5-diphenyl-1H-imidazole is reported. It is through one pot synthetic protocol by the reaction of mole quantities 4-methoxy aniline (1 mmol, 0.123g), benzil (1 mmol, 0.210g), ammonium acetate (1 mmol, 0.75g) and 4-nitro-benzaldehyde (1mmol, 0.150g) in glacial acetic acid medium. The IR, ¹H-NMR, ¹³C NMR spectra, SEM and EDAX were used in structure elucidation. The crystal structure reveals π electron delocalization in the molecule. Inter- and intra-molecular hydrogen bonds, C-H... π interactions and H...H contribute to the stability of structure.

Graphical Abstract



Keywords: 1-(4-methoxyphenyl)-2-(4-nitrophenyl)-4,5-diphenyl-1H-imidazole, Synthesis, Single Crystal Structure, SEM, EDAX, Hirshfeld Surface, C-H... π interactions