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Synthesis, Characterization and DFT Calculation of Naphthalene-Based Crystal Structure with Pyridylimine-Binding Units

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Naphthalene-based structures and imine systems have diverse multidisciplinary applications, including the assembly of cyclophanes, helicates, dimers, trimmers, and grids[1-3]. The authors synthesized a compound using 1,6-diaminonaphthalene and pyridine-2-carbaldehyde through refluxing in extra-pure ethanol. The resulting crystal was characterized using single crystal X-ray diffraction. The article describes a crystal structure consisting of two pyridylimine-binding units linked to a 1,5-naphthalene. The structure is connected by C-C, C-H, and π-stacking interactions to form a three-dimensional structure. The crystal has four units with two orientations in each unit face of the unit cell and belongs to the monoclinic space group P2(1)/c. The structure was fully verified through infrared examination. The infrared examination showed a strong peak at 1288 cm^{-1} due to aromatic amine stretching frequency, two medium peaks related to CH_2 and CH_3 deformation, and a medium peak at 1472 cm^{-1} corresponding to the symmetric bending vibration of the CH_2 group. The absence of hydrogen atoms bonded to highly electronegative atoms in the structure suggests that its physical and chemical properties, such as melting point, boiling point, solubility, and reactivity, are not affected. The absence of hydrogen bonding interactions can have various effects in different applications. Additionally, we included computational results for NMR, Raman, and charge distribution using the Gaussian software.

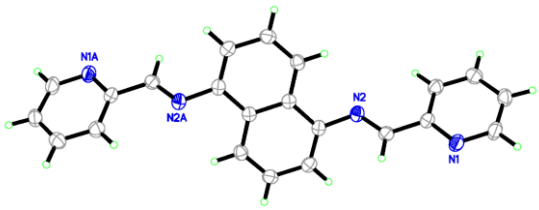


Fig.1.Molecular structure of Ligand

Keywords: Schiff-base, Aromatic, weak interaction, Crystal structure, DFT.

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