Characterization of crystal structure of 4-(4H-1,2,4-Triazol-4-yl) phenol prepared by hydrothermal

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Abstract: 4-(4H-1,2,4-Triazol-4-yl)phenol (compound I) as a triazol aromatic compound was obtained by the reaction diformylhydrazine and p-aminophenol in dimethylformamide (DMF) under hydrothermal condition. The crystal structure of this compound was determined by FT-IR spectroscopy, NMR, elemental analysis and single crystal X-ray diffraction method. Crystallographic data for I was collected at 298 K. The synthesized compound has been crystallized in orthorhombic system with pbcn space group and a = 10.9373(15) Å, b = 7.4539(10) Å, c = 18.530(3) Å, Z = 8. The crystal structure was solved by direct methods and refined by full-matrix least squares to final values of $R_1 = 0.0682$ and $wR_2 = 0.1361$ with 1328 reflections. There are various types of supramolecular interactions including hydrogen bonding and π-π stacking in the crystal structure of I. These interactions play important role in the expansion of 3D network of compound I.

Keywords: triazolphenol; orthorhombic; single crystal X-ray diffraction; supramolecular interactions.