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Different classical hydrogen –bonding patterns in two imidazole derivatives (N-(tert-butyl)-2-(4-nitrophenyl)imidazo[1,2-a]pyrazin-3-amine and N-(tert-butyl)-2-(2-nitrophenyl)imidazo[1,2-a]pyridin-3-amine)

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Abstract : The title compounds, $C_{16}H_{17}N_5O_2$ in (I) and $C_{17}H_{18}N_4O_4$ in (II), are imidazole derivatives in which the imidazole moiety is fused with a piperdine ring system in (I), and with an benzene ring system in (II). The compound I, crystallized in the triclinic space group p1- with two molecules in a unit cell and compound II, crystallizes in a monoclinic in a C-centered lattice with eight molecules in the unit cell. According to single-crystal x-ray data, intra (C-H…N 3.397(3)) Å and intermolecular hydrogen bonds C-H…O 3.397(3)Å are formed between C-H groups of the imidazole cycle and O atoms of the paramagnetic moieties. The intermolecular H-bonds connect the molecules forming chains along the c-axis. Moreover, there are short intermolecular contacts between the O atoms (3.97)Å and between the O and C atoms (3.98)Å of the nitrophonyl moiety within the chain. Anti-bacterial study reveals that complexes are better anti-microbial agents than three Schiff base due to bacterial cell penetration by chelation.
Keywords : imidazole, pyridine, Crystal Structure, hydrogen bonding.

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