

## Molecular and crystal structures, vibrational studies and quantum chemical calculations of 3 and 5-nitroderivatives of 2-amino-4-methylpyridine.

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The crystal structures of 2-amino-4-methyl-3-nitropyridine (I), 2-amino-4-methyl-3,5-dinitropyridine (II) and 2-amino-4-methyl-5-nitropyridine (III) have been determined. The compounds crystallize in the monoclinic  $P2(1)/n$ , triclinic  $P-1$  and monoclinic  $C2/c$  space groups, respectively. These structures are stabilized by a combination of  $N-H\cdots N$  and  $N-H\cdots O$  hydrogen bonds and exhibit layered arrangement with a dimeric  $N-H\cdots N$  motif in which the molecular units are related by inversion centre. The molecular structures of the studied compounds have been determined using the DFT B3LYP/6-311G(2d,2p) approach and compared to those derived from X-ray studies. The IR and Raman wavenumbers have been calculated from the optimized geometry of monomers and dimers formed in the unit cell and compared to the experimental values obtained from the spectra.

### Słowa kluczowe

2-amino-4-methyl-3-nitropyridine, 2-amino-4-methyl-3, 5-dinitropyridine, 2-amino-4-methyl-5-nitropyridine, IR and Raman spectra, crystal structure, Intra-and intramolecular hydrogen bonds

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