

Crystal structure, vibrational and optic properties of 2-N-methylamino-3-methylpyridine N-oxide : its X-ray and spectroscopic studies as well as DFT quantum chemical calculations.

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The crystal and molecular structure and physicochemical properties of 2-N-methylamino-3-methylpyridine N-oxide (MA3MPO) have been studied. MA3MPO was synthesized from 2-amino-3-methylpyridine by several steps to form colorless crystals suitable for crystallographic analysis. The data reveal that MA3MPO crystallizes in the monoclinic space group $P2_1/n$. The studied compound contains a nearly flat triply substituted pyridine skeleton whose structure is stabilized by an intramolecular N–H···O hydrogen bond. The N-oxide molecules are connected together by weak C–H···O hydrogen bonds, an acceptor of which is the oxygen atom from the N-oxide group. This leads to creation of two-dimensional network of hydrogen bonds. Its IR, Raman, UV–Vis and luminescence spectra have been measured and analyzed on the basis of DFT and NBO quantum chemical calculations in which the B3LYP/6-311++G(d,p) approach was applied. The distribution of the electron levels in the studied compound has been analyzed in terms of the possibility of its participation in the ligand-to-lanthanide ion energy transfer.

Słowa kluczowe

2-N-Methylamino-3-methylpyridine N-oxide, Synthesis, Crystal structure, IR, Raman, UV–Vis and luminescence spectra, NBO and DFT calculations

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