Thione-thiol tautomerism in new 4-methyl-3-nitopyridine derivative in the solid state – X-ray, electron absorption and emission, IR and Raman studies discussed in term of quantum chemical DFT calculations

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Streszczenie

Theoretical and experimental studies of new 4-methyl-3-nitropyridine-2-thione and its thiol tautomer were synthesized and characterized by means of structural and spectroscopic studies. X-ray diffraction, IR, Raman, UV–VIS and emission spectra were measured and analyzed. The quantum chemical DFT calculations were applied in the analysis of the obtained results. The effect of the temperature change on the structural and spectroscopic properties was studied. The vibrational characteristics and dynamical properties of the □-S-H and □=*S* type compounds are discussed where □ is a heterocyclic ring. The results of structural and spectroscopic studies were used to find a diagnostic tool on the structure of thione and thiol forms and their optic properties.

Słowa kluczowe

Thione-thiol tautomerism, 4-methyl-3-nitropyridine-2-thione/2-thiol, Crystal structure, Ir and raman spectra, UV–VIS spectra, Luminescence

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