Synthesis and physicochemical properties of the methyl-nitro-pyridine-disulfide: X-ray, NMR, electron absorption and emission, IR and Raman studies and quantum chemical calculations

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Streszczenie

The methyl-nitro-pyridine-disulfide derivative [2,2 - disulfanodiylbis(6-metyl-3-nitropyridine)] was syn- thesized and characterized by means of structural and spectroscopic measurements. On the basis of X-ray diffraction studies, it was found that the studied compound crystallizes in the centrosymmetric mono- clinic space group P2 1 /n (Z = 2). The disulfide C-S-S-C bridge links two identical fragments formed by pyridine rings substituted with methyl and nitro groups. Such a structure was confirmed by 1 H and 13 C NMR studies as well as IR, Raman, UV–VIS and emission spectra. Quantum chemical DFT calculations were applied in the analysis of the obtained results. The vibrational characteristics were reported and dynamical properties of this moiety were discussed. A full set of the normal modes characteristic for the disulfide bridge was identified and assigned to the respective IR and Raman bands. The results of structural and spectroscopic studies were used to find the dependence between the conformation of the φ-S-S- φsystem and its optic properties. The experimental electron and emission spectra were analyzed in terms of the calculated singlet and triplet states that allowed assigning the unique spectral pattern originating from the electrons of the C-S-S-C bridge system.

Słowa kluczowe

Methyl-nitro-pyridine disulfide, NMR, Spectroscopic studies, Electron excited states

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