

Excited-state forms of 2-methylamino-6-methyl-4-nitropyridine*N*-oxide and 2-butylamino-6-methyl-4-nitropyridine*N*oxide.

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Streszczenie

Excited-state quantum chemical calculations of two 2-alkylamino-6-methyl-4-nitropyridine *N*-oxides are presented. Several different calculation methods and different basis sets were used, which all lead to similar results, although the precise values of excited-state energies and excited-state dipole moments differ. All methods used predict that in the S_1 excited state four types of isomers occur. In three cases, these excited-state local energy minima correspond to ground-state isomers, and these all have a $\pi\pi^*$ character. The fourth excited-state minimum, which we denote L^* , does not have a corresponding ground-state isomer and has an $n\pi^*$ character. This isomer is stable and plays an important role in understanding the photophysics of these molecules. In addition, we also calculated barriers between these excited-state minima, using predefined reaction pathways. The theoretical results derived in this Article are confronted with experimental data from earlier papers.

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