ROTATIONALLY RESOLVED ELECTRONIC SPECTROSCOPY OF BIOMOLECULES IN THE GAS PHASE. MELATONIN.

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Rotationally resolved electronic spectra of the A and B bands of melatonin have been analyzed using an evolutionary strategy approach. From a comparison of the *ab initio* calculated structures of energy selected conformers to the experimental rotational constants, the A band could be shown to be due to a gauche structure of the side chain, while the B band is an anti structure. Both bands show a complicated pattern due to a splitting from the three-fold internal rotation of the methyl rotor in the N-acetyl group of the molecules. From a torsional analysis we additionally were able to determine the barriers of the methyl torsion in both electronic states. The electronic nature of the lowest excited singlet state could be determined to be ^1L_b (as in the chromophore indole) from comparison to the results of *ab initio* calculations.