Manipulation of electronically excited states of indole

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The electronic origin bands of several singly substituted indole derivatives were investigated using rotationally resolved electronic spectroscopy [1-5]. From the experimentally determined transition dipole moment orientation in combination with high level *ab initio* calculations the electronic nature of the electronically excited states was elaborated. Following the nomenclature of Platt [6] the lowest excited singlet states can be characterized as an L_a or L_b state, depending on the orientation of the transition dipole moment.
Starting with the substituent at the biologically important position 5 at the indole chromophore the influence of different substituents on the photophysics of indole could be explored.
Based on a broad range of substituents exerting different effects to the indole chromophore it could be shown that mesomeric effects have a greater impact on the energetic nature of the excited states than inductive effects.
Recently, these investigations were expanded by changing the position of the substituent at the chromophore.
A thorough understanding of these influences may allow for a systematic manipulation of the electronically excited states.

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