$C_{2\mathrm{v}}$-TOP INTERNAL ROTATION IN THE HIGH-RESOLUTION UV SPECTRA OF WEAKLY BOUND COMPLEXES: I. THE MODEL OF A C_{2v} TOP – C_{s} FRAME INTERNAL ROTATION.[a]

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In rotationally resolved UV spectra of weakly bound complexes, different effects of large amplitude motions are observable. In complexes with molecules such as nitrogen or water, these molecules can undergo internal rotation and the spectra are split into different subbands due to rotation–internal rotation interactions. In contrast to internal rotation cases with a symmetric top, the elements of the kinetic energy tensor depend on the internal rotation angle in these complexes where the top is of symmetry $C_{2\mathrm{v}}$. A semirigid internal rotor model consisting of a rigid frame of C_{s} symmetry and one internal rotor of C_{2v} symmetry was developed for internal rotation problems in microwave spectroscopy by A. Bauder *et al.* (Mol. Phys. **15** (1968), 597). This method has been extended in order to fit and simulate rotationally resolved UV spectra.
In Part I, the theory of the model will be presented; applications of this model will be discussed in Part II.

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