

STATES AND TRANSITION IN FLOPPY COUPLED ROTOR MODELS

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It is well known that when the dipole moment of a symmetric rotor lies along the main symmetry axis it gives a comparatively simple spectrum. However, in a floppy molecular system made of two coupled rotors there can be reorientation of axes resulting in a multiplicity of structure and a more complex spectrum. This is further complicated by level splitting depending sensitively on coupling strength. We have investigated effects on levels and the spectrum over different types of coupling and a range of coupling strength. States range from a weakly coupled angular momentum bases to more Born-Oppenheimer-like states, which we label as Body-Oriented-Angular or BOA-constricted bases. Analogous effects were first investigated by Seaton, Fano, Jungen, Harter and Patterson in simpler cases involving a diatomic rotor coupled to an electron varying between high Rydberg orbitals in a low l -uncoupling limit and l -uncoupled molecular orbitals. Here we consider two full quantum rotors between analogous limits of coupling. Considerations of molecular symmetry and goodness of quantum labels also play an important role in sorting out the dynamics and spectral effects.