THEORETICAL STUDIES OF INTERNAL ROTATION FOR AN ASYMMETRIC 'TOP'

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For internal rotation in 3-fold tops, the internal axis system (IAS) has been a great convenience because the vibrational angular momentum is constant and is directed along a single axis. A procedure for finding an IAS for the general asymmetric top-asymmetric frame case will be given. This Procedure is an existence proof that such an axis system can be found. Once the IAS is found, details will be given on how the Matthieu equation can be solved and how the results can be described as a Fourier series. A useful alternative to the IAS is an axis system obtained by rotating away from the IAS by a constant amount (independent of the torsional angle) so as to position the frame in a more convenient orientation. For this reduced axis system (IAS), a Matthieu equation can also be used as a basis except that the kinetic energy for the Matthieu solution only contains contributions from the a component of the vibrational angular momentum. Expectation values for other operators including contributions from the b component of the vibrational angular momentum are deferred to the full diagonalization of the rotation-vibration Hamiltonian. Examples of internal rotation systems incorporating these ideas will be given.

Time required: 15 min
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