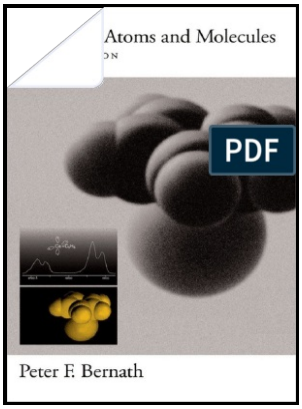
Tables for the rigid asymmetric rotor - transformation coefficients from symmetric to asymmetric bases and expectation values of Pz2, Pz4, and Pz6

U.S. Dept. of Commerce, National Bureau of Standards - Simplified methods for the computation of asymmetric rotor energy levels and line strengths



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Angular momentum (Nuclear physics)Tables for the rigid asymmetric rotor - transformation coefficients from symmetric to asymmetric bases and expectation values of Pz2, Pz4, and Pz6
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Simplified methods for the computation of asymmetric rotor energy levels and line strengths

The 2D case is shown in Figure 1.

Classification of rigid rotors

For a linear molecule the separation of lines in the rotational spectrum can be related directly to the moment of inertia of the molecule.

Symmetric and Asymmetric Components

Substituting these results into the expression for the energy term of a symmetric rotor on the previous page gives: Note that this is precisely the same expression as for a spherical rotor.

Simplified methods for the computation of asymmetric rotor energy levels and line strengths

Explicit line strength formulas for low rotational quantum numbers and approximation formulas for nearly symmetric rotors are given.

Linear and Asymmetric Rotors

In this case the lines that do not rotate principal are the C- D orthogonal pair and maximum rotation is in the x- y orientation. Therefore, the asymmetric displacement tensor can be rewritten The rotation is not a tensor of second order, but a vector? The form of the reduced energy matrices used by previous authors as starting point for computations has been modified by a simple algebraic reduction in a manner which permits substantial savings in the amount of numerical work required for the calculation of rigid rotor energy levels and centrifugal distortion corrections.

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