

The Gateway Hamilton Operator: Theory and Practice

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I shall explain the gateway Hamiltonian method [1-3] and demonstrate its applicability by calculation of vibrational energy levels.

In particular, it shall be explained and numerically demonstrated that:

- Even when expressed in terms of curvilinear internal coordinates, the gateway kinetic energy operator (KEO) is of an expression nearly identical with the Eckart-Watson operator [4].
- It obviates the need for differentiation of the matrix rotating into the Eckart frame.
- It allows construction of an Eckart ro-vibrational KEO without rotation.
- It leads to defining optimal Eckart displacements.

References

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