

Vibrational Quantum Dynamics of Complex Molecular Systems with Numerical Kinetic Energy Operators in Generalized Coordinates Using a Method to Obtain the Eckart Hamiltonian and The Equations of Motion of a Highly Deformable Polyatomic System in Terms of Generalized Coordinates

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Received date: September 05, 2023; Accepted date: September 15, 2023; Published date: September 22, 2023

Citation: Alireza Heidari, (2023). Vibrational Quantum Dynamics of Complex Molecular Systems with Numerical Kinetic Energy Operators in Generalized Coordinates Using a Method to Obtain the Eckart Hamiltonian and The Equations of Motion of a Highly Deformable Polyatomic System in Terms of Generalized Coordinates, *Journal of Clinical Anatomy*, 2(5) DOI:10.31579/2834-5134/033

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A delivered collectively (as one) change of the entire (nonrelativistic) molecular Hamiltonian from Cartesian to generalized coordinates has been done. The change is pretty standard and may be carried out for random vibrational (twist/bend/alternate the form) actions in addition to most selections of shifting axes systems. Eckart's axis conference (and by that/in that way Hamiltonian) is discussed as an instance of application. The trade of the translational--rovibronic (non-relativistic) Hamiltonian from cartesian to generalized coordinates by means of the (related to tiny, weird actions of atoms)-mechanical route organized and listed in the previous paintings has been accomplished for linear molecules. The translational-rovibronic Hamiltonian for a non-linear polyatomic molecule is received/made from by means of using the Schrödinger equation in tensor shape and using the Eckart conditions (figuring out/identifying the nuclear- (stable basic shape on which bigger things may be constructed) rotational (numbers that change/matters that trade)). the existing derivation is an added collectively (as one) entire and thorough one with the aid of a (associated with tiny, bizarre actions of atoms)-mechanical pathway and is very different from (made of unconnected pieces) previous derivations thru a classical-intermediate route. The method offered presents a company concept-based photo of the character of the trade

and the origin of coupling phrases, and avoids mathematical problems with their residue of being unknown. the best form of the full (the first-class of something it's turning wanting to hold turning) operators is likewise received/made from (associated with tiny, weird actions of atoms) robotically [1-114].

Acknowledgement:

This study was supported by the Cancer Research Institute (CRI) Project of Scientific Instrument and Equipment Development, the National Natural Science Foundation of the United States, the International Joint BioSpectroscopy Core Research Laboratory (BCRL) Program supported by the California South University (CSU), and the Key project supported by the American International Standards Institute (AISI), Irvine, California, USA.

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