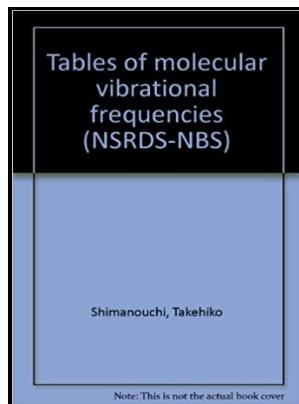


Tables of molecular vibrational frequencies.

National Bureau of Standards - Molecular Spectroscopic Data



Description: -

Vibrational spectra -- Tables. Tables of molecular vibrational frequencies.

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Notes: Supersedes and extends data in, Tables of molecular vibrational frequencies, NSRDS-NBS-6, Pt 1; NSRDS-NBS-11, Pt 2; and NSRDS-NBS-17, Pt 3.

This edition was published in 1972



Filesize: 63.61 MB

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12: Vibrational Spectroscopy of Diatomic Molecules

On the other hand, there is no difficulty to record the atomic trajectory in theoretical simulations.

Table 1 from An evaluation of harmonic vibrational frequency scale factors.

The quantities under study include vibrational frequencies of 7 isotopomers, isotopic shifts, as well as absorption intensities. Moeller-Plesset perturbation theory is employed to improve the accuracy of static mean field computations in mol. As this print on demand book is reprinted from a very old book, there could be some missing or flawed pages, but we always try to make the book as complete as possible.

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However, the problem that complicates the matter is that the equilibrium positions of atoms in vibration are constantly changing because of the overall rotating, random tilting, and drifting motions of the molecule in a vacuum.

Efficiently Calculating Anharmonic Frequencies of Molecular Vibration by Molecular Dynamics Trajectory Analysis

For convenience, representative line antenna temperatures are listed for a typical astronomical source for each transition, and the references are cited for the laboratory and astronomical literature that have been employed. Using root-mean-square errors from the values in the large databases, we find that scaling reduces errors in zero-point energies by a factor of 2. Finally, the vibrational fingerprint of the excitation energy of a more complex mol.

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