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Chapter 7 - Symmetry and Spectroscopy - Molecular Vibrations - p. 8 - vib NUH  $\nu(k, Q, k)$   $k \Phi = g^{1/2}$  with  $\sum = -i i i Q U e^{2 2 1} h$  w and  $h k k w g =$  Hermite polynomials:  $H_0(z) = 1$   $H_1(z) = 2z$   $H_2(z) = 4z^2 - 2$   $H_3(z) = 8z^3 - 12z$   $H_4(z) = 16z^4 - 48z^2 + 12$  Note: even for even  $\nu, k$ , odd for odd  $\nu, k$ . Therefore  $( ) \Gamma \Phi \dots$

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where  $k$  is the bond force constant and  $m$  is the reduced mass for two nuclei of masses  $m_1$  and  $m_2$ .  $= \frac{1}{\frac{1}{m_1} + \frac{1}{m_2}}$  This yields the quantized vibrational level scheme shown in Figure 5.1 A. Because transitions between the  $v = 0$  and  $v = 1$  levels dominate in infrared or Raman spectroscopy, the harmonic

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Τμήμα Χημείας - Πανεπιστήμιο Κρήτης

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## **Τμήμα Χημείας - Πανεπιστήμιο Κρήτης**

A. Symmetry is when a shape or object has two completely identical sides that are either facing each other or are around an axis. A line of symmetry is the line that divides the two identical ...

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This substitution gives the force constants  $k_r$ ,  $k_R$ ,  $k_{rr}$ , and  $k_{rR}$  in N/m units and the bending constants  $k_d$  and  $k_{dd}$  in units of N m. Rotational levels and transitions. The vibrational-rotational energy levels for a linear molecule are similar to those for a diatomic molecule and, to a good approximation, are given in  $\text{cm}^{-1}$  units by the sum ...

## **Chem435. Physical Chemistry Laboratory. Lab9. IR**

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## **Spectroscopy**

Symmetry & IR Spectroscopy. One of the most importance applications of IR spectroscopy is structural assignment of the molecule depending on the relationship between the molecule and observed IR absorption bands. Every molecule is corresponding to one particular symmetry point group. Then we can predict which point group the molecule is ...

## **Infrared: Theory - Chemistry LibreTexts**

K. Veera Reddy, "Symmetry and Spectroscopy of Molecules", New Age International (P) Limited, Publishers (1997).

M.S.Gopinathan & V. Ramakrishnan, "Group Theory In Chemistry", Visal Publications (2000).

## **Group Theory (Reference) : Inorganic Chemistry Virtual Lab ...**

Molecular symmetry in chemistry describes the symmetry

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present in molecules and the classification of molecules according to their symmetry. Molecular symmetry is a fundamental concept in chemistry, as it can be used to predict or explain many of a molecule's chemical properties, such as its dipole moment and its allowed spectroscopic transitions. To do this it is necessary to classify the ...

## **Molecular symmetry - Wikipedia**

Molecular Symmetry and Spectroscopy deals with the use of group theory in quantum mechanics in relation to problems in molecular spectroscopy. It discusses the use of the molecular symmetry group, whose elements consist of permutations of identical nuclei with or without inversion.

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Rotational-vibrational spectroscopy is a branch of molecular spectroscopy concerned with infrared and Raman spectra of molecules in the gas phase. Transitions involving changes in both vibrational and rotational states can be abbreviated as rovibrational (or ro-vibrational) transitions. When such transitions emit or absorb photons (electromagnetic radiation), the frequency is proportional to ...

## **Rotational-vibrational spectroscopy - Wikipedia**

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While genuine symmetry is an ideal state, pseudosymmetry represents a continuum of distortion from the ideal to the asymmetric state. It will be shown that symmetry in molecular structure manifests itself by affording degenerate frequency spectroscopic and diffraction signals from equivalent molecular subunits.

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