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Chapter 7 - Symmetry
and Spectroscopy -
Molecular Vibrations -
p. 8 - vib NUH v (k Q k)
k $\Phi = g 1/2$ with $\Sigma = -$
i i i Q U e 2 2 1 h w and
h k k w g = Hermite
polynomials: $H_0(z) = 1$
 $H_1(z) = 2z$ () 4 2 1 H
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$2z = z - H(z) 8z3 12z$

$3 = -(\) 16 4 48 2 12$

$H 4 z = z - z +$ Note:
even for even v k , odd
for odd v 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 .
$$m = \frac{m_1 m_2}{m_1 + m_2}$$
 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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**CHAPTER 5 -
SYMMETRY AND
VIBRATIONAL
SPECTROSCOPY 5.1**

...

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the symmetry of the excited state will be the direct product of the irreducible representation for $\psi_1(2)$ and $\psi_3(1)$. For example, in the point group C_{4v} , v_1 has symmetry e and v_3 has symmetry a_2 . By performing the calculations listed above, it is determined that $\psi_1(2)$ has $(a_1 + b_1 + b_2)$ symmetry:

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Combination Bands, Overtones and Fermi Resonances ...

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,

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to a good approximation, are given in cm^{-1} units by the sum ...

Experiment 9. Rotational-Vibrational Spectroscopy ...

2.1: Group Theory: Theory; 2.2: Understanding Character Tables of Symmetry Groups; 2.3: Group Theory; 2.4: Infrared - Theory Infrared (IR)

spectroscopy is one of

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the most common and widely used spectroscopic techniques employed mainly by inorganic and organic chemists due to its usefulness in determining structures of compounds and identifying them.

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undergraduate-level text introduces vibrational and electronic spectroscopy, presenting applications of group theory to the interpretation of UV, visible, and infrared spectra without assuming a high level of background knowledge. 200 problems with solutions. Numerous illustrations. "A uniform and consistent

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In vibrational spectroscopy, transitions are observed between different vibrational states. In a fundamental vibration, the molecule is excited from its ground state ($v = 0$) to the first excited state ($v = 1$). The symmetry of the

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ground-state wave function is the same as that of the molecule.

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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

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absorb photons
(electromagnetic
radiation), the
frequency is
proportional to ...

Rotational-vibration al spectroscopy - Wikipedia

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