

Name: _____

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Please answer any 6 questions, showing all calculations - 25 points each, 150 total.

- List the symmetry elements of the following molecules and name the point groups to which they belong: (a) ammonia (NH_3), (b) trans-dichloroethene ($\text{CHCl}=\text{CHCl}$), (c) nitrobenzene ($\text{C}_6\text{H}_5\text{NO}_2$), (d) tetrahydrofuran ($\text{C}_4\text{H}_8\text{O}$), (e) PCl_5 (trigonal bipyramidal structure).
- Determine the CH and CN bond lengths in HCN given the following rotational constants $B(^1\text{H}^{12}\text{C}^{14}\text{N}) = 44.316 \text{ GHz}$ and $B(^2\text{H}^{12}\text{C}^{14}\text{N}) = 36.208 \text{ GHz}$. For a linear A–B–C molecule, $I = m_A R_{AB}^2 + m_C R_{BC}^2 - (m_A R_{AB} - m_C R_{BC})^2 / (m_A + m_B + m_C)$
- Write out a group multiplication table for the C_{3v} point group.
- Calculate the symmetry species of the irreducible representation of rotation, vibration and translation of the molecule BH_3 in the point group D_{3h} . Under the C_3 and S_3 operations, the character is 0 and -2 respectively rather than the ± 1 you might predict using a vector model. Show which of these modes are IR and Raman active. What would be the symmetry species of the symmetric stretch of all three H atoms (+5 bonus)?

D_{3h}	E	2C_3	3C_2	σ_h	2S_3	$3\sigma_v$	
A_1'	+1	+1	+1	+1	+1	+1	$x^2 + y^2, z^2$
A_2'	+1	+1	-1	+1	+1	-1	R_z
E'	+2	-1	0	+2	-1	0	$(x, y), (x^2 - y^2, xy)$
A_1''	+1	+1	+1	-1	-1	-1	
A_2''	+1	+1	-1	-1	-1	+1	z
E''	+2	-1	0	-2	+1	0	$(\text{R}_x, \text{R}_y), (yz, zx)$

- Which of the following molecules show a pure rotational Raman spectrum (a) CH_2Cl_2 , (b) CH_3CH_3 , (c) SF_6 , (d) N_2O .
- The rotational constant for CO is 1.9314 cm^{-1} in the ground state and 1.6116 cm^{-1} in the excited state. By how much does the internuclear distance change as a result of this transition?
- Describe what is meant by the term "anharmonicity" as applied to vibrational energy levels of a diatomic molecule.
- Which of the following molecules N_2 , NO , O_2 , C_2 , F_2 , and CN would you expect to be (a) stabilized by the addition of an electron to form AB^- , (b) the removal of an electron to form AB^+ ?
- What information does the term symbol $^1\text{D}_2$ provide about the angular momentum of an atom?
- Consider a particle in a cubic box, what is the degeneracy of the level which has $14/3$ times the energy of the lowest energy state?