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The Unshifted Atom-A Simpler Method of Deriving Vibrational Modes of Molecular Symmetries

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ABSTRACT

The infrared and Raman spectroscopy are widely utilized to study molecular structures. Of great interest is the great interest is the striking correlation between the molecular geometry and the infrared and Raman spectra of simple molecules and ions. This incredible correlation tends to be shadowed by deep theoretical and mathematical principles such that a good number of scholars are denied the joy of appreciating the correlation between molecular symmetry and infrared and Raman spectra. The 'unshifted atom' method presents a highly simplified approach based on basic knowledge of symmetry elements and the effect of symmetry operations on molecular geometries to determine the number of unshifted atoms (US_a). Inserting the Cartesian coordinates(X,Y,Z) on an unshifted atom and applying symmetry operations, the contributions to the character (X_{so}) by the symmetry operations are obtained. A simple multiplication of the numbers of unshifted atoms (US_a) in a point group with the Corresponding numbers of (X_{so}) generates a REDUCIBLE REPRESENTATION from which the VIBRATIONAL MODES of a molecule/ion are deduced. Examples of different molecular geometries have been presented to illustrate the simplicity, flexibility and viability of the method.

Key words: Vibrational modes, Molecular symmetries, Spectroscopy.

INTRODUCTION

Infrared spectroscopy has been extensively used for both military and civilian purposes since its discovery by Herschel¹ in 1800. In chemistry, it has been utilized for the characterization of molecular structures of simple and complex molecules²⁻⁶. From the study of infrared spectra of a vast range of molecules, scientists have been able to design a chart of characteristic absorption frequencies of molecular functional groups⁷. Such an infrared chart is extremely useful in predicting the type of functional groups from the infrared spectrum of an unknown sample or the expected absorption ranges of a sample whose molecular formula is known.

Symmetry and group theory principles have been utilized to interpret the bonding and the infrared and Raman spectra mainly of simple molecules^{2,8-11}. In the case of bonding, the molecular bonds are regarded as the basis set or vectors from which a Reducible Representation is generated¹². This is then decomposed into appropriate Irreducible Representations from bonding information is derived. But in the case of infrared or Raman Spectroscopy, three Cartesian coordinates (x, y, z) are inserted on each atom of the molecule or ion under consideration^{8-9,11,13}. The reason for this is that a molecule possesses Translational, Rotational and Vibrational energies. These are resolved into x, y and z vectors for each of the atom in the molecule. This set of x, y and z coordinates form the BASIS SET for generating irreducible representation

For instance, if CH, is being considered for bonding, only 4 vectors are taken into account whereas if IR or Raman Spectroscopy is being considered, 3x5 =15 (3xN, N = number of atoms in the molecule) Cartesian coordinates will be considered. The use of 3N vectors is not only cumbersome but also the level of mathematical theory accompanying the explanation of IR and Raman spectroscopy⁸⁻¹³ tend to frighten or deny the joy of enjoying the correlation between molecular symmetry and the corresponding IR/Raman spectra of molecules/ions for chemists who may not have a good depth of physical chemistry. Although the concept of unshifted atom has briefly been used before¹⁴⁻¹⁵ no detailed account has been given. The aim of this article is to introduce in details a condensed simple unshifted atom method of deriving the expected number of IR/Raman peaks from the symmetry of simple molecule or ion. Hence, this paper hopes to popularize the unshifted atom method so as to put to rest the cumbersome conventional and traditional method of dealing with the system of Cartesian coordinates attached to every atom in given molecule or ion to obtain vibrational modes.

METHODS

The method involves first determining the point group of the molecule or ion. The second step is to determine the number of un shifted atoms (US_a) when acted upon by symmetry operations namely, E, σ i, C_n and S_n). The final important step is to determine the character by the three coordinates on an unshifted atom. This is illustrated in the diagram below.





IDENTITY (E) OPERATION

Contribution to character will be [(+1) + (+1) + (+1)] = 3.

This can more appropriately be derived from a matrix format as shown below.

$$E \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$
$$E \boxed{1 \quad 0 \quad 0}$$

$$X_E = 3$$

It is not necessary to be using matrices to derive the character of a symmetry operation as this can be easily extracted by inspection of the signs of the Cartesian coordinates after the effect of the symmetry operation.

POINT OF INVERSION (i)

$$(X,Y,Z)$$
 i operation $(-X,-Y,-Z)$

Hence, the contribution to character is [(-1) + (-1) + (-1)] = -3.

PLANE OF SYMMETRY (s) OPERATION

$$(X,Y,Z) \xrightarrow{\sigma_{XY} \text{ operation}} (X,Y,-Z)$$

. .

Contribution to character will be [(+1) +(+1)+(-1)] = +1. In terms of the contribution to character, $\sigma_{xy} = \sigma_{xz} = \sigma_{yz} = +1$.

C_n OPERATION

Consider rotation of $c_{_{\!\!n}}$ clockwise through an angle θ



 \downarrow Rotation through θ, clockwise by c



Z is perpandicular

The vector components contributions to the original directions are $X \cos\theta$ by X in the original x-axis and Y $\cos\theta$ by Y vector in the y-axis.

Hence, the contributions to the character by X-vector is $\cos\theta$, and the contribution to the







S_n OPERATION

We also know that $\boldsymbol{S}_{_n} = ~\boldsymbol{C}_{_n} \, \boldsymbol{x} \, \boldsymbol{\sigma}_{_h}.$ Therefore, ~~ operations.

its operation can be broken into the following operations.



Table 1. Summary of symmetry operation contribution to character table.

Contrik	oution to charac	ter,(χ so) b	y unshifted	atom (US _a))		
E	Cn Sn i						
+3	1+2cosq	-	1+2cosq	-3	}	+1	
	n=	2	3	4	6		
	C _n	C ₂ =-1	C ₃ =0	C ₄ =1	C ₆ =2		
	S _n		S ₃ =-2	S ₄ =-1	S ₆ =0		

Examples

Let us apply the above concepts to selected molecules/ions to illustrate the power of the method. Initially, we can apply the conventional method of using all the Cartesian coordinates on a simple molecule such as water, H_2O . Later on we will apply the simpler method for comparison. Consider H_2O as an illustration in Fig.1.



Fig.1: The Cartesian coordinate system of H₂O

Point group is C_{2v} . The identity symmetry operation, E leaves all the 9 Cartesian coordinates unchanged. Hence we insert 9 under E in the C_{2v} character table. The C_2 symmetry operation completely shifts all the Cartesian coordinates on the two H atoms. These contribute zero to the C_{2v} character table. However, $C_2(X,Y,Z)$ on the O atom gives rise to , (-X, -Y, +Z). The net contribution to the character of C_2 operation becomes, [(-1)+(-1)+(+1)] = -1. The symmetry operation $\sigma_{\chi_Z}(X, Y, Z)$ for the O atom, we get (X, -Y, Z) giving a net contribution to the σ_{χ_Z} character of +1. This is the same for each of the two H atoms. Hence, σ_{χ_Z} the overall contribution to the character is +3. Similarly, σ_{χ_Z} will have a contribution to character of +1. The entire set of numbers generated by symmetry operations are known as REDUCIBLE REPRESENTATIONS, $\Gamma_{_{3N}}$. This is shown in table 2.

Table 2: The	Reducible	Representati	on of H ₂ O an	nd the $C_{_{2v}}$	Character 7	Table

C _{2v}	Ε	C ₂	σ_{xz}	σ_{yz}
Г _{ЗN}	9	-1	3	1
5		h=4		
A1	1	1	1	1
A ₂	1	1	-1	-1
B1	1	-1	1	-1
B ₂	1	-1	-1	1

The Reducible representation is then decomposed into Irreducible representations using the following reduction formula.

 $N_{IR} = 1/h \Sigma X_R X_{IR}$

 N_{IB} = Number of irreducible representations,

h = order of the group(the sum of symmetry operations),

 X_{R} = character of reducible representation,

 X_{IR} = character of irreducible representation.

Applying the above formula, we get:

$$\begin{split} \mathsf{N}_{\mathsf{A1}} &= \frac{14}{9}[9.1+(-1).1+3.1+1.1]=3\\ \mathsf{N}_{\mathsf{A2}} &= \frac{14}{9}[9.1+(-1).1+3.(-1)+1.(-1)]=1\\ \mathsf{N}_{\mathsf{B1}} &= \frac{14}{9}[9.1+(-1).(-1)+3.1+1.(-1)]=3\\ \mathsf{N}_{\mathsf{B2}} &= \frac{14}{9}[9.1+(-1).(-1)+3.(-1)+1.(1)]=2\\ \Gamma_{\mathsf{3N}} &= 3\mathsf{A_1}+\mathsf{A_2}+3\mathsf{B_1}+2\mathsf{B_2} \end{split}$$

Selection rules

 Γ_{TBANS} = Transform as X, Yand Z

 $\begin{array}{ll} \Gamma_{\text{ROT}} = & \text{Transform as } R_x \text{ , } R_y \text{, and } R_z \\ \text{Hence, } \Gamma_{\text{TRANS}} = & A_1 + B_1 + B_2 \text{ since they transform} \\ \text{as } X, Y \text{ and } Z \text{ and } \Gamma_{\text{ROT}} = & A_2 + B_1 + B_2 \\ \text{since they transform as } R_x \text{ , } R_y \text{, and } R_z \text{.} \\ \text{Since, } \Gamma_{3N} = \Gamma_{\text{TRANS}} + \Gamma_{\text{ROT}} + \Gamma_{\text{VIB}} \\ \text{then } \Gamma_{\text{VIB}} = \Gamma_{3N} - \Gamma_{\text{TRANS}} - \Gamma_{\text{ROT}} \text{ Thus,} \\ \Gamma_{\text{VIB}} = & (3A_1 + A_2 + 3B_1 + 2B_2) - (A_1 + B_1 + B_2) \text{-} (A_2 + B_1 + B_2) \\ \text{giving us,} \\ \Gamma_{\text{VIB}} = & 2A_1 + B_1 \end{array}$

Selection rules

IR _{ACTIVE} transform as x, y, and z RM_{ACTIVE} transform as Products of x, y, and z. IR_A = Infrared active and RM_A = Raman active. Since A₁ + B₁ symmetries are IR and Raman active, we expect to see 3 PEAKS in both IR and Raman spectra. These are (cm⁻¹) 3657, 1595 and 3756. Applying the simpler method on H₂o.

AB₂ system

Table 3: Derivation of Reducible Representation of H₂O using shorter and simpler method.

C _{2v}	E	C ₂	σ_{xz}	σ _{yz}
USa	3	1	3	1
Xso	3	-1	1	1
Гзм	9	-1	3	1

This means that determining the number of unshifted atoms (US_a) by each of the symmetry operations and the contribution to the character(χ_{SO}) by each symmetry operation and multiplying them easily produces (Γ_{3N}). Thus, $\Gamma_{3N} =$ (US_a) X (χ_{SO}). Then, Γ_{3N} can be decomposed into Irreducible representations in the usual way as described above.

Let us take a few more examples to illustrate the power of the method.

AB, SYSTEM

Consider $BF_{_3}$ as shown in Fig.2. This has a $D_{_{3h}}$ point group.



Fig. 2: The coordinate system of BF₃

The starting point is to generate the number of unshifted atoms (US_a) by each symmetry operation of the D_{3h} point group. Under E operation, all atoms of BF₃ are not shifted. Hence, we enter 4 under E operation. The number of unshifted atoms for C₃, C₂, σ_h , S₃, and σ_h are 1, 2, 4, 1 and 2

respectively. The corresponding contribution to character(χ_{so}) by each symmetry operation obtained from Table 1 are also recorded. The product of US_a, χ_{so} and the corresponding number of symmetry operations, produces the row of Reducible Representation Γ_{sn} . These are given in Table 4.

for generating vibrational symmetries for BF ₃											
D _{3h}	Е	2C ₃	3C ₂	$\sigma_{_{h}}$	2S ₃	3 σ _v					
US_a χ_{so} Γ_{aN}	4 3 12	1 0 0	2 -1 -6	4 1 4	1 -2 -4	2 1 6					

Table 4: Derivation of Reducible Representation

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Using the reduction formula, $\Gamma_{_{3N}}$ is the decomposed into Irreducible Representation symmetries which comprise of $\Gamma_{_{TRANS}}$, $\Gamma_{_{ROT}}$ and $\Gamma_{_{VIB}}$. The symmetries of $\Gamma_{_{TRAN}}$ and $\Gamma_{_{ROT}}$ are extracted from $D_{_{3h}}$ character table. They are then subtracted from $\Gamma_{_{3N}}$ leaving $\Gamma_{_{VIB}}$ symmetries. Applying the selection rules to $\Gamma_{_{VIB}}$ symmetries, we can deduce how many are IR active or Raman active. In the case of BF $_{_3}$, we expect to observe 3 peaks in IR spectrum and 3 peaks in Raman spectrum with 2 peaks in common. This is what is observed* and is given in Table 5.

Г _{зN}	= A1' + A2' + 3E' + 2 A2" + E"
Γ_{TRANS}	= E' + A2"
$\Gamma_{\rm ROT}$	= A ₂ ' + E"
Γ_{VIB}	$= A_1' + 2E' + A2''$
IR _A	= $\sqrt{\sqrt{-3}}$ peaks
RM _A	$= $ $$ \rightarrow 3 peaks

Table 5: IR and Raman Spectral data² of BF₃

BF₃(g)	A1'	A2"	Ε'	Ε'
cm'	888	718 IR₄	1505 IR₄	482 IR₄
	RM _A	RM _A	RM _A	

2 in common

As can be seen from tables 6 and 7, the theoretical model is consistent with the experimental data.

AB₄ SYSTEM TETRAHEDRAL (T_d) Example

The reason why this method is so easy is that it eliminates the burden of visualizing the set of all coordinates on the atoms within the molecule/ ion. It only focuses on the unshifted atom(s) by a symmetry operation (US_a) and the corresponding contribution to the character (χ_{SO}) by the symmetry operation. When this approach is applied to CH₄ shown in Fig.3. the results obtained are given in Table 6.



Fig. 3: Tetrahedral geometry of CH₄

Table 6. Derivation ofReducible Representation for generatingvibrational symmetries for CH₄

Е	8C ₃	3C ₂	6S ₄	$6 \sigma_{d}$
5	2	1	1	3
3	0	-1	-1	1
15	0	-3	-6	18
	E 5 3 15	E 8C ₃ 5 2 3 0 15 0	E $8C_3$ $3C_2$ 5 2 1 3 0 -1 15 0 -3	E $8C_3$ $3C_2$ $6S_4$ 5 2 1 1 3 0 -1 -1 15 0 -3 -6

Table 7: IR and Raman Spectral data² of CH₄

CH4	A ₁	Е	T ₂	T ₂
cm⁻¹ IR	2917	1534	3019 √	1306 √
RM _A				\checkmark

AB₅ SYSTEM

The application of the method to PF_{5} shown in Fig. 4 gives us the results shown in tables 8 and 9.



Fig. 4: The trigonal bipyramid of PF_{s}

Table 8: Derivation of Reducible Representation for generating vibrational symmetries for $PF_{_{5}}$

D _{3h}	E	2C,	3	3C ₂	σ _h	2S ₃		3 σ _v
US	6	3		2	4	1		4
X	3	0		-1	1	-2		1
Г_м	18	0		-6	4	-4		12
Γ_{3N} Γ_{TDANC}	2A ₁ '	A ₂ '		4E' E'	3A2" A2"	2E"		
Γ_{pot}		A, ^D			2	E"		
	2A ₁ '	2		3E'	2A2"	E"		E pooko
RM _A	\checkmark				V			6 peaks
			3 C	OMMON				
		Table 9): IR and Ra	aman Spect	ral data ² of Pl	5		
PF₅(g)	A ₁ '	A ₁ '	A ₂ ''	A ₂ ''	Ε'	E'	Ε'	E''
	017	640	044	EZE	1006	E 0 0	200	E 1 4

AB, molecules including one lone pair

 $\sqrt{}$

IR_A RM



The unshifted atom method indicates that BrF_{5} molecule is expected to show 6 and 9 peaks in IR and Raman respectively with 6 peaks in common. This is shown in Table 10 and is consistent with the experimental data in Table11.

Fig. 5: The square pyramidal geometry of BrF5.

							•		
BrF₅	A ₁	A ₁	A ₁	B ₁	B ₁	B ₂	Е	Е	Е
cm⁻¹ IR.	682 √	570 √	365 √	535	281 √	312 √	644 √	414	237
RM _A				\checkmark				\checkmark	\checkmark

Table 9: IR and Raman Spectral data² of BrF₅

Table 10: Derivation of Reducible Representation for generating vibrational symmetries for BrF₅

C _{4v}	E	2C ₄	C ₂	2σ _v	$2\sigma_{d}$	
US	6	2	2	4	2	
X _{so}	3	1	-1	1	1	
Γ_{3N}	18	4	-2	8	4	
Γ _{3N}	4A,	A ₂	2B,	B ₂	5E	3N=18
Γ_{TBANS}	A	-	·	_	E	
Γ_{BOT}		A ₂			E	
Γ_{VIB}	3A,	-	2B,	B ₂	3E	3N-6=12
IR				-	\checkmark	6 peaks
RM _A	\checkmark			\checkmark	\checkmark	9 peaks

More examples

Due to the viability of the method, let us apply it to a few more molecular geometries.

The theoretical and experimental data are given in tables 10 and 11.

ISOMERS OF N₂F₂

Gan point group

Fig. 6: The geometry of trans-N₂F₂

C _{2h}	E	C ₂	i	σ _h	
$\begin{array}{l} \text{US}_{a} \\ \text{X}_{so} \\ \Gamma_{3N} \\ \Gamma_{TRANS} \\ \Gamma_{TRANS} \\ \Gamma_{ROT} \\ \Gamma_{VIB} \\ \text{IR}_{A} \\ \text{RM}_{A} \end{array}$	4 3 12 4A _g A 3Å _g √ no peaks in	0 -1 0 2B _g 2B _g	0 -3 0 2A _u A _u √	4 1 4 2B _u 2B _u √	3N=12 3N-6=6 3peaks 3 peaks

Table 10: Derivation of Reducible Representation for generating vibrational symmetries for PF5

Trans-N ₂ F ₂ (I)	\mathbf{A}_{g}	\mathbf{A}_{g}	\mathbf{A}_{g}	B _u	B _u	A _u		
cm ⁻¹	1010 √	1522 √	600 √	990	423	364		
RM _A					\checkmark	\checkmark		
no peaks in common, total 6 peaks								

Table 11: IR and Raman Spectral data² of Trans N₂F₂

The data clearly shows that a molecule with a centre of symmetry, the IR spectrum and Raman spectrum have no peaks in common.

CIS ISOMER

The theoretical and experimental data for the cis-N $_{\rm 2}{\rm F}_{\rm 2}$ are given in Tables 12 and 13.



Fig. 7: The geometry of $cis-N_2F_2$

Table 12: Derivation of Reducible Representation fo
generating vibrational symmetries for Cis- N ₂ F ₂

C _{2v}	E	C ₂	σ _{xz}	σ _{γz}	
$\begin{array}{l} {\sf US}_{\sf a} \\ {\sf X}_{\sf so} \\ {\sf \Gamma}_{\sf 3N} \\ {\sf \Gamma}_{\sf TRANS} \\ {\sf \Gamma}_{\sf ROT} \\ {\sf \Gamma}_{\sf VIB} \\ {\sf IR}_{\sf A} \\ {\sf RM}_{\sf A} \end{array}$	4 3 12 4A ₁ A ₁ 3A ₁ √ 5 peaks in co	0 -1 0 $2A_2$ A_2 mmon	0 1 0 2B ₁ B ₁ B ₁	$\begin{array}{c} 4\\ 1\\ 4\\ 4B_2\\ B_2\\ B_2\\ 2B_2\\ \\ \\ \end{array}$	5 peaks 6 peaks

Cis-N ₂ F ₂ (I)	A ₁	A ₁	A ₁	B ₂	B ₂	A ₂
cm ⁻¹ IR	896 √	1525 √	341 √	952 √	737 √	550
RM _A	√ 5 peaks	√ in 'common	\checkmark	\checkmark	\checkmark	\checkmark

Table 13: IR and Raman Spectral data² of Cis-N₂F₂

It is also interesting to note that the less symmetrical a molecule is, the more peaks are observed.

The A-X stretchng frequencies

The vibrational stretching frequencies are extremely useful in characterizing molecular structures. The stretching modes refer to the stretch between two atoms (A-X). A-X can refer to two atoms such as C-H, C=O, C-CI, N-H and C-S.

Let us take H_2CO molecule as an illustration. It has a C_{2v} geometry as shown below.

Using the 'unshifted atom method', it is predicted that 6 peaks to be observed. Furthermore, two C-H stretching frequencies and one CO stretching frequency are expected. This is in agreement with the experimental data. This is summed up in Table 14.



Fig. 8: The geometry of H₂CO

			-		-	
C _{2v}	E	C ₂	Γ_{xz}	$\Gamma_{\rm YZ}$		
US	4	2	4	2		
X	3	-1	1	1		
Γ_{3N}	12	-2	4	2		
Γ _{an}	4A,	A ₂	4B,	3B,		
Γ_{TRANS}	A,	2	B, ່	B		
Γ_{BOT}		A ₂	B	B		
Γ_{VIB}	3 A,	-	2 B,	B ₂		
IR					6 peaks	
RM _A	\checkmark		\checkmark	\checkmark	6 peaks	
C-H	2	0	2	0		
$\Gamma_{\rm CH}$	A ₁		B ₁		2 peaks	
C=O	1	1	1	1		
Γ_{co}	A ₁				1 peak	
H ₂ CO ³	2783	1746	1500	2843	1249	1167
_	A ₁	A ₁	A ₁	B ₁	B ₁	B ₂
C-H		-	-		-	-
C=O		\checkmark				

Table 14: Derivation of Reducible Representation for generating vibrational symmetries for H₂CO as well the spectral data of H₂CO

Metal carbonyls

Consider the C=O stretching frequencies. Hence use C=O bonds as the as the BASIS SET.

The C=O stretching frequency can be used for structural analysis of carbonyls. This is illustrated by the examples of Ni(CO)₄, and the distinction of the isomers of $MX_2(CO)_4$. The results are given in Tables 15-17.



Fig. 9: The geometry of Ni(CO)₄

T _d	E	8C ₃	3C ₂	6S ₄	$6 \sigma_{d}$
$\begin{array}{c} CO \\ \Gamma_{\infty} \\ \Gamma_{\infty} \\ IR_{A} \\ RM_{A} \end{array}$	4 4 A₁ √	1 8 T₂ √ √	0 0	0 0	2 12 1 peak 2 peaks

Table 15: Derivation of Reducible Representation for generating vibrational symmetries for C=O stretching frequencies of $Ni(CO)_4$





Table 16: Derivation of Reducible Representation for generating vibrational symmetries for C=O stretching symmetries of Trans- $MX_2(CO)_4$

D_{4h}	Е	2C ₄	C ₂	2C2 ^D	2C ₂ ^{DD}	i	$2S_4$	σ_{h}	2 σ _v	2σ _d
со	4	0	0	2	0	0	0	4	2	0
Γ_{co}	4	0	0	4	0	0	0	4	4	0
Γ _{co} IR,	$A_{_{1g}}$	$B_{_{1g}}$	E_{u}							1 peak
RM _A	√ no pea	√ ks in con	nmon							2 peaks

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Fig. 11: The geometry of $cis-MX_2(CO)_4$

Table 17: Derivation of Reducible Representation for generating vibrational symmetries for C=O stretching symmetries of $Cis-MX_2(CO)_4$

C _{2v}	E	C ₂	σ _{xz}	σ _{γz}	
CO Ã _{co} IR _A RM _A	4 2A₁ √ √ all in cor	0 B₁ √ √	$\begin{array}{c} 2 \\ \mathbf{B}_{2} \\ \sqrt{2} \\ \sqrt{2} \\ \sqrt{2} \end{array}$	2	4 peaks 4peaks

It should be noted that when considering stretching frequencies, the filtration of $\Gamma_{\rm TRANS}$ and $\Gamma_{\rm ROT}$ is not involved. on

CONCLUSION

This paper aims to appeal to many readers of science so as to greatly appreciate the correlation

between the symmetry and point group of a molecule/ion on one hand and its infrared/Raman spectrum on the other. The molecule could be as simple as C_2H_4 or P_4 to more complex ones such as C_6H_6 or C_{60} . It is hoped that from various backgrounds such biology, biochemistry, chemistry, physics, mathematics and geology among others will enjoy reading this article.

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REFERENCES

- 1. http://en.wikipedia.org/wiki/Infrareddownloaded -16-01-2012
- K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination compounds, Willey Interscience, New York, 4th Edition, 1986.
- T. Shimanouchi, Tables of Molecular Vibrational Frequencies, United States Department of Commerce, National Bureau of Standards, 172
- J. Coates, Interpretation of Infrared Spectra, A Practical Approach, Encyclopedia of Analytical Chemistry, John Wiley and Sons Ltd, Chichester, 10851(2000).
- http://www.organicchemistry.com/tag/ infrared-spectroscopy/-downloaded-03-01-2012
- 6. P.J. Larkin, Infrared and Raman Spectroscopy, Elsevier, 69(2011).
- http://student.ccbcmd.edu/~cyau1/ 203%20Appen%2004%20IR% 20Absorptions%20Part%20I%202008.pdfdownloaded -16-01-2012.

- F. A. Cotton, Chemical Applications of Group Theory, John Wiley and Sons, New York, 3rd Edition, 304(1990).
- R. S. Drago, Physical Methods in Chemistry, Saunders College Publishing, Philadelphia, 153 (1977).
- D.F. Shriver and P. W. Atkins, Inorganic Chemistry, Oxford 11. University Press, 3rd Edition, 135(1999).
- P. Atkins, Physical Chemistry, W. H. Freeman and Company, New York, 6th Edition, 485(1998
- 12. See reference 8, p.204.
- Alan Vincent, Molecular Symmetry and Group Theory, John Willey and Sons Ltd, 121(1981).
- http://www.unf.edu/~michael.lufaso/ chem3610/Inorganic_Chapter4.pdfdownloaded -16-01-2012.
- http://www.b-u.ac.in/sde_book/ msc_phychem.pdf-downloaded-16-01-2012.