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Identification of optically active vibrational modes of columbite AB_2O_6 using correlation method

ABSTRACT

In the modern era, the examination of molecular structure heavily relies on the application of infrared and Raman spectra within crystalline structures. These methodologies are essential in understanding the arrangement of atoms within molecules and the internal forces governing them. An essential aspect of this analysis involves identifying vibrational modes that can be detected optically. The correlation method is employed to establish rules for selecting these vibrational modes, both in crystals and molecules, through a systematic calculation process that aids in predicting their activity in Infrared (IR) and Raman spectra. The correlation method utilizes group theory to determine which vibrational modes are spectroscopically active in crystals. In our research, our aim is to employ this method to identify the irreducible representations and determine the IR and Raman active vibrational modes of orthorhombic AB_2O_6 compounds within the Pbcn space group. By conducting comprehensive group theory calculations, our objective is to elucidate the spectroscopic properties using the correlation method.

Keywords: *Correlation method, spectroscopy, group theory, columbite-type structure*

1. INTRODUCTION

Due to the large application of IR and Raman modes of crystals, it is useful to know the active spectroscopic modes. The correlation method is employed to establish the selection criteria for both crystals and molecules. The correlation method is preferred over the conventional selection rules due to their time-consuming and laborious procedure. For the molecular structures, it is easy to derive the vibrational modes using selection rules but for the crystals it becomes cumbersome. Lately, there has been an increasing fascination with the investigation of AB_2O_6 oxides, mainly due to their wide-ranging applications and their prevalence in the natural environment.

As a result, there is a pressing demand for comprehensive investigations into their structural characteristics[1], properties, and lattice arrangements. The AB_2O_6 structure represents a class of semiconductor metal oxides that have demonstrated potential for photocatalysis. Columbite-structure AB_2O_6 Oxides are attractive for various applications due to its excellent dielectric properties, as well as its photocatalytic and organic catalytic activities. Typically, the columbite-type structure crystallizes in the orthorhombic space group Pbcn[2].

AB_2O_6 Oxides ($A=Mn^{2+}$, $B=V^{5+}$, here) crystallize in the columbite structure. The cations of A and B are located in the center of the octahedra are surrounded by six oxygen atoms while the AO_6 and BO_6 octahedra share the edges, forming independent zigzag chains. This sequential situation repeats as ABBABB octahedral layers as the chains are connected by sharing corners in order to the AO_6 chain-BO_6 chain-BO_6 chain [3].

In this ongoing dialogue, we have explored AB_2O_6 oxides in their orthorhombic phase with the Pbcn space group, employing the correlation method [4,5].

Through meticulous calculations, we have successfully anticipated the Raman and infrared activities, as well as their associated vibrational modes. Prior to delving into specifics, it is essential to grasp the following terms:

1.t^{γ} = the quantity of movements within the specific site species γ, which can vary between 0 and 3. This data is accessible through the character table.

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2.R^{γ} = no. of rotations in site species, it may also have values 0,1,2, or 3 and represented as R_x, R_y, R_z.

3.f^{γ} = the degree of freedom for vibrational and is obtained from $f^{\gamma} = nt^{\gamma}$; n represent no. of equivalent atoms, ions, or molecules in site species.

4.$F_R{}^{\gamma}$ = the degree of freedom for rotational modes inherent in each species γ within an equivalent set of ions or molecules, determined by $F_R{}^{\gamma} = n.R^{\gamma}$

5. a_{γ} = the degrees of freedom provided by each site species γ to a factor group ξ, with a_{γ} derived from $a_{\gamma} = f^{\gamma}/\sum_{\xi} C_{\xi}$

6.C_{ξ} = the multiplicity of species γ within the factor group, as detailed in Table 1. At times, it demonstrates its relationship to the species within the site group.

Table 1: Types of Species and their Corresponding C_{ξ} Values [4]

Species	Value of C_{ξ}
A	1
B	1
E	2
F	3
G	4
H	5

Within the realm of factor group species, irreducible equation provides a clear insight into the tally of lattice vibrations within a corresponding group of similar atoms. Additionally irreducible-representation symbolized as' Γ,' to emphasize that, for the crystal precisely indicates the quantity of lattice vibrations existing within each category of the factor group. It's noteworthy that the irreducible-representation 'Γcrystal' encompasses both acoustical and optical vibrations.

Entire irreducible-representation is obtained by adding irreducible-representations of each equivalent set of atoms [6]

To specifically isolate the optical vibrations, this process entails subtracting the irreducible-representation of acoustical vibrations, resulting in the representation denoted as 'Γoptical':

$$\Gamma optical = \Gamma crystal - \Gamma acoustical$$

A step-by-step discussion of correlation using MnV_2O_6 in orthorhombic structure with space group Pbcn [7] as an example is done here.

Factor group analysis of orthorhombic MnV_2O_6 in Pbcn structure

2. CRYSTALLOGRAPHIC INFORMATION AND SPACE GROUP IDENTIFICATION

The first step of the correlation method is to find the space group and Bravais lattice. The space group and Bravais lattice must be known to get the crystallography of the compound. Here we have the Pbcn space group and orthorhombic crystal structure for the present compound MnV_2O_6.

Z(No of molecules in unit cell)/ L P (lattice points)= Z^B

MnV_2O_6 is four formula unit crystal belonging to space group Pbcn. MnV_2O_6 has 4 equivalent Mn atoms, 8 atoms of Vanadium, and 24 Oxygen atoms in the Bravais unit cell.

Site symmetry

The site symmetry for MnV_2O_6 is as follows:

$$D_{2h}^{14} : 2C_i\,(4);\ C_2(4);\ C_1(8)$$

The number enclosed within the parentheses of site symmetry [9] signifies the count of equivalent atoms that possess that specific site symmetry. For instance, there are four equivalent atoms on sites labeled as C_2, and eight equivalent atoms on sites denoted as C_1. The site C_i can accommodate up to four equivalent atoms, and the coefficient '2' indicates the existence of two distinct types of C_i sites within the unit cell, given in Table 2. It's possible to have atoms on either, both, or neither site within the crystal. It's crucial to verify that the quantity of equivalent atoms corresponds to the capacity stipulated by the site symmetry.

Table 2. Site symmetry and Wycoff position of atoms [8,9]

Atom	Wycoff position	Site symmetry
Mn	4c	$C_2(4)$
V	8d	$C_1(8)$
O_1	8d	$C_1(8)$
O_2	8d	$C_1(8$
O_3	8d	$C_1(8)$

Site $C_2(4)$ is filled with Manganese, while site $C_1(8)$ accommodates both Vanadium and Oxygen. Site $2C_i$ (4) remains unoccupied. The Wyckoff positions are specified as follows: 4c for Manganese, 8d for Vanadium, and 8d each for Oxygen sites labelled as O_1, O_2, and O_3.

Correlation

The subsequent stage involves aligning the site group with the factor group through correlation. Utilizing the correlation table [4], each species within the site group is matched with its counterpart in the factor group. This correlation aids in identifying the species responsible for lattice

vibrations in the crystal, facilitating the prediction of infrared and Raman activity [10,11]. This correlation process establishes the connection between each species in the site group and its corresponding species in the factor group [12].

3. APPLICATION OF CORRELATION METHOD TO MANGANESE ATOMS IS AS FOLLOWS

Manganese is situated at site $C_2(4)$, which accommodates four atoms. According to the character table of site C_2, displacements along the x, y, and z axes are associated with site species A and B. The proper correlation method for relating the C_2 site symmetry to the D_{2h} factor group, as indicated by the Wyckoff description, is based on the presence of Manganese Mn atoms located at the Wyckoff site 4c, where 'c' is associated with the site correlation column C_2 (y) within D_{2h}^{14}. Referring to the correlation table, we can establish that A corresponds to A_g, B_{2g}, A_u, B_{2u}, while B corresponds to B_{1g}, B_{3g}, B_{1u}, and B_{3u}. Therefore, following table 3 & 4 utilizes the correlation method for this purpose.

Table 3. Character Table for C_2 Point Group [4]

C_2	E	C_2		
A	1	1	T_z; R_z	α_{xx}, α_{yy}, α_{zz}, α_{xy}
B	1	-1	T_x, T_y; R_x R_y	α_{xz},, α_{yz}

Table 4: Correlation for the Lattice Vibrations of Manganese in the MnV_2O_6 Crystal in the Pbcn Phase between the Site Group C_2 and Factor Group D_{2h}

n	$f^\gamma = nt^\gamma$	t^γ	Site species $\gamma(C_2)$	correlation	Factor group $\xi(D_{2h})$	C_ξ	a_ξ	species
4	4	T_z (1)	A	→	A_g	1	1	
				→	B_{2g}	1	1	
				→	A_u	1	1	
				→	B_{2u}	1	1	
8	T_x, T_y (2)		B	→	B_{1g}	1	2	
				→	B_{3g}	1	2	
				→	B1u	1	2	
				→	B_{3u}	1	2	

Using the relation, $f^\gamma = a_\gamma \sum_\xi C_\xi$,we can determine the value of the degrees of freedom provided by each site species γ to a factor group a_γ

There are two possible values of f^γ,$f^\gamma = 4$, $f^\gamma = 8$

By employing the equation $f^\gamma = a_\gamma \sum_\xi C_\xi$,

For $f^\gamma = 4$, we find that $4 = 4a_\gamma$, which leads to $a_\gamma = 1$

For $f^\gamma = 8$, the equation $8 = 4a_\gamma$ yields $a_\gamma = 2$.

Utilizing the equation $\Gamma = \sum a_\xi C_{\xi:}$, for the irreducible-representation for the Manganese atom, $\Gamma_{Mn} = A_g + B_{2g} + A_u + B_{2u} + 2B_{1g} + 2B_{3g} + 2B_{1u} + 2B_{3u}$. However, this irreducible-representation encompasses both acoustical and vibrational modes. To isolate the vibrational modes, the acoustic modes must be subtracted.

The correlation method is applied to Vanadium atoms as follows:

The vanadium atom lies on site $C_1(8)$ as shown in Table 5.

Table 5. Character table for the Symmetry Group C_1[4]

C_1	E	
A	1	T_x,T_y,T_z

From the character table of site C_1, translations along x, y, and z corresponds to site A, and from the correlation table A corresponds to A_g, B_{1g}, B_{2g}, B_{3g}, A_u, B_{2u}, B_{1u}, B_{2u}, B_{3u} According to the character table of site C_1, Displacements along the x, y, and z axes are attributed to the site species A. According to the Wyckoff description, the appropriate correlation method to link the C_1 site symmetry to the D_{2h} factor group relies on the existence of Vanadium atoms situated at the Wyckoff site 8d,

where 'd' is associated with the site correlation column C_2 (y) within D_{2h}^{14} . Referring to the correlation table, we can establish that A corresponds to A_g, B_{1g}, B_{2g}, B_{3g}, A_u, B_{2u}, B_{1u}, B_{2u}, B_{3u} Therefore, following Table 6 utilizes the correlation method for this purpose.

Table 6. Correlation for the Lattice Vibrations of Vanadium in the MnV_2O6 Crystal in the Pbcn Phase between the Site Group C_1 and Factor Group D_{2h}

n	$f^\gamma = nt^\gamma$	t^γ	Site species $\gamma(C_1)$	Correlation	Factor group species $\xi(D_{2h})$	C_ξ	a_ξ
8	24	Tx, Ty, Tz	A	→	Ag	1	3
					B1g	1	3
					B2g	1	3
					B3g	1	3
					Au	1	3
					B1u	1	3
					B2u	1	3
					B3u	1	3

Using the relation, $f^\gamma = a_\gamma \sum_\xi C_\xi$,we can determine the value of the degrees of freedom provided by each site species γ to a factor group a_γ

For f^γ =24, 24=8a_γ, we get a_γ =3

Using $\Gamma=\sum a_\xi C_\xi$, irreducible-representation for Vanadium atom

$$\Gamma_V = 3A_g + 3B_{1g} + 3B_{2g} + 3B_{3g} + 3A_u +$$
$$+ 3B_{2u} + 3B_{1u} + 3B_{2u} + 3B_{3u}$$

The correlation method is applied to all three types of Oxygen atom is O_1, O_2 & O_3 atoms as follows:

From the character table of site C_1, translations along x,y, and z corresponds to site A, and from the correlation table A corresponds to A_g, B_{1g}, B_{2g}, B_{3g}, A_u, B_{2u}, B_{1u}, B_{2u}, B_{3u} According to the character table of site C_1, displacements along the x, y, and z axes are associated with site species A.

Table 7. Correlation concerning the lattice vibrations of oxygen atoms O_1, O_2, and O_3 within the MnV_2O_6 crystal in the Pbcn phase, comparing Site Group C_1 with Factor Group D_{2h}

n	$f^\gamma = nt^\gamma$	t^γ	Site species $\gamma(C_1)$	Correlation	Factor group species $\xi(D_{2h})$	C_ξ	a_ξ
8	24	T_x, T_y, T_z	A	→	Ag	1	3
					B1g	1	3
					B_{2g}	1	3
					B3g	1	3
					Au	1	3
					B1u	1	3
					B2u	1	3
					B3u	1	3

The proper correlation method for relating the C_1 site symmetry to the D_{2h} factor group, as indicated by the Wyckoff description, is based on the presence of Oxygen atoms located at the Wyckoff site 8d, where 'd' is associated with the site correlation column C_2 (y) within D_{2h}^{14} . Referring to the correlation table, we can establish that A corresponds to A_g, B_{1g}, B_{2g}, B_{3g}, A_u, B_{2u}, B_{1u}, B_{2u}, B_{3u} Therefore, table 7 gives the correlation method for this purpose**.**

Using the relation, $f^{\gamma} = a_{\gamma} \sum_{\xi} C_{\xi}$,we can determine the value of the degrees of freedom provided by each site species γ to a factor group a_{γ}

For f^{γ} =24,24=8a_{γ}, we get a_{γ} =3.

Using $\Gamma=\sum a_{\xi} C_{\xi}$,we can determine the irreducible representations .Since O_1,O_2,O_3 lies on same Wycoff site 8d , irreducible representations for each Oxygen atom will be same .Therefore, Irreducible-representation for Oxygen O_1, O_2 & O_3

$$\Gamma_{O1,\,O2,\,O3} = 3A_g + 3B_{1g} + 3B_{2g} + 3B_{3g} + 3A_u + 3B_{2u} + 3B_{1u} + 3B_{2u} + 3B_{3u}$$

The overall representation of the crystal, denoted as Γcrystal, can be determined by summing the irreducible representations for each group of equivalent atoms i.e. Mangnese Mn, Vanadium V, three types of Oxygen O_1, O_2, O_3

$$\Gamma_{crystal} = \Gamma_{Mn} + \Gamma_{V} + \Gamma_{O1} + \Gamma_{O2} + \Gamma_{O3}$$

$$\Gamma_{crystal} = 13A_g + 13B_{2g} + 14B_{1g} + 14B_{3g} + 13A_u + 13B_{2u} + 14B_{1u} + 14B_{3u}$$

Acoustic modes are recognized within the factor group due to their similarity in character to translational motion. The acoustical mode representation is denoted as $\Gamma_{acoustical}$ and comprises B_{1u}, B_{2u}, and B_{3u} as indicated in the character table for D_{2h}, which assigns translations to these modes.

The representation $\Gamma_{acoustical}$ consists of B_{1u}, B_{2u}, and B_{3u} as these modes are associated with translations according to the character table of D_{2h} (Table 8).

$$\Gamma_{acoustical} = B_{1u} + B_{2u} + B_{3u}$$

In the realm of vibrational spectroscopy, crystals exhibit vibrational modes that can be categorized into irreducible representations of their respective point groups. Acoustical modes represent the translational motions of the crystal and typically have zero frequency. They are included in the irreducible representations [14] but are not physically meaningful for vibrational spectroscopy. To analyze the relevant vibrational modes, you need to remove these acoustical modes from the irreducible representations.

$$\Gamma_{optic} = \Gamma_{crystal} - \Gamma_{acoustical} = 13A_g + 13B_{2g} + 14B_{1g} + 14B_{3g} + 13A_u + 12B_{2u} + 13B_{1u} + 13B_{3u}$$

Table 8. Character Table for D_{2h} Point Group [4]

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	σ(xy)	σ(zx)	σy(z)	Rot./trans.	Polarization
A_g	1	1	1	1	1	1	1	1		$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}$
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	α_{xy}
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y	α_{xz}
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	α_{yz}
A_u	1	1	1	1	-1	-1	-1	-1		
B_{1u}	1	1	-1	-1	-1	-1	1	1	T_z	
B_{2u}	1	-1	1	-1	-1	1	-1	1	T_y	
B_{3u}	1	-1	-1	1	-1	1	1	-1	T_x	

By using character table & correlation table used for D_{2h} space group, infrared and Raman activity can be anticipated. In addition to characters, the character table contains two columns. the vibrational modes represented by symbols Tx, Ty, and Tz belong to irreducible representations that exhibit the same transformation properties as x, y, and z, and they are also active in the infrared spectrum. Another additional column contains various binary combinations of coordinates from which the Raman activity of vibrations can be obtained.

Therefore, we find that Raman active modes are - A_g, B_{1g}, B_{2g}, and B_{3g} and Infrared active modes are A_u, B_{1u}, B_{2u}, and B_{3u}. with A_u representing an inactive mode. These results are presented in tabular form in Table 9. These findings are also reported in the works of Dapeng Xu et al. [15] and Tyagi et al. [16], thereby validating our results.

Table 9. D_{2h} Character Species, Raman and Infrared Active, Acoustical and Silent Modes in the MnV_2O_6 Crystal in phase Pbcn obtained by Correlation Method

Factor Group Species	Translational species	Acoustical mode species	Γcryst	Γvib	Infrared activity	Raman polarization tensor	Raman activity
A_g			13	13		α_{xx}, α_{yy}, α_{zz}	√
B_{1g}			14	14		α_{xy}	√
B_{2g}			13	13		α_{xz}	√
B_{3g}			14	14		α_{yz}	√
A_u			13	13			
B_{1u}	T_x	1	14	13	√		
B_{2u}	T_y	1	13	12	√		
B_{3u}	T_z	1	14	13	√		

4. CONCLUSION

The application of group theory calculations to orthorhombic MnV_2O_6 has facilitated the identification of spectroscopically active vibrational modes within the crystal This calculation involves correlating the site symmetry of each atom within the crystal with the factor group of the crystal. This correlation is crucial in deriving an irreducible-representation for the vibrational modes of the crystal, enabling the separate examination of each mode. The results obtained can be reinforced by accounting for both the atomic degrees of freedom within the crystal and the vibrational degrees of freedom. This comprehensive analysis ensures the accuracy and reliability of the calculated vibrational mode. These results hold significant value, as they can be applied to the study of the microstructure of both the molecules and crystals, shedding light on their dynamic behavior and structural properties. Such insights are essential for understanding the fundamental characteristics of materials and their potential applications.

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IZVOD

IDENTIFIKACIJA OPTIČKI AKTIVNIH VIBRACIJSKIH REŽIMA KOLUMBITA AB_2O_6 KORIŠĆENJEM METODE KORELACIJE

U modernoj eri, ispitivanje molekularne strukture se u velikoj meri oslanja na primenu infracrvenog i Ramanovog spektra unutar kristalnih struktura. Ove metodologije su neophodne za razumevanje rasporeda atoma unutar molekula i unutrašnjih sila koje njima upravljaju. Suštinski aspekt ove analize uključuje identifikaciju vibracionih modova koji se mogu optički detektovati. Korelacioni metod se koristi za uspostavljanje pravila za odabir ovih vibracionih modova, kako u kristalima tako i u molekulima, kroz sistematski proces proračuna koji pomaže u predviđanju njihove aktivnosti u infracrvenom (IR) i Raman spektru. Korelacioni metod koristi teoriju grupa da odredi koji su vibracioni modovi spektroskopski aktivni u kristalima. U našem istraživanju, naš cilj je da upotrebimo ovu metodu za identifikaciju nereducibilnih reprezentacija i određivanje IR i Raman aktivnih vibracionih modova ortorombskih AB2O6 jedinjenja unutar Pbcn prostorne grupe. Sprovođenjem sveobuhvatnih proračuna teorije grupa, naš cilj je da razjasnimo spektroskopska svojstva korišćenjem metode korelacije.

Ključne reči: *Korelacioni metod, spektroskopija, teorija grupa, struktura tipa kolumbita*

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