MODES OF ATOMIC VIBRATION IN THE FOURTEEN BRAVAIS LATTICES

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Introduction

In the first paper in this symposium, Sir C. V. Raman has discussed the normal modes of vibration of a crystal lattice, and has come to the conclusion that, in a normal mode, the atoms in adjacent cells must vibrate either in the same or opposite phases. In other words, starting from any atom, if one proceeds to an equivalent atom in the next cell by any one of the three primitive translations, the latter atom must vibrate with a phase either the same as or opposite to that of the former. If we represent the ratio of the amplitudes of atoms in adjacent cells along the three principal directions by α, β and γ, then these can take only the values $+1$ or -1. Also, the value of α, β or γ must be the same for *all* the non-equivalent atoms in the unit cell, if the equations of motion are to be satisfied. Hence, in the general study of the vibrations of crystal lattices, we may, as a first step, apply these ideas to determine the nature of the vibrations for the fundamental Bravais lattices.

It is, no doubt, true that few crystals possess the simple Bravais lattices for their structure; but any crystal can be built out of a number of such lattices interpenetrating one another. Then, the values of α, β and γ will be the same for every one of the non-equivalent atoms in the unit cell, and the vibrations will pertain to the same type as those for the simple lattice. Obviously, each mode of the simple lattice will be split up into p modes, if there are p atoms per unit cell. These will have to be determined by making use of the condition that all the p atoms in the cell must vibrate in either the same, or opposite phases, and also that the relative phases of the atoms must be identical in every cell. But a consideration of the relative phases alone is not sufficient in a general case, and one has to take into account the force system, etc. However, in some simple cases with a relatively small number of atoms occupying special positions in the lattice, a consideration of phase relations alone may suffice to enable the modes to be described more or less completely.

It is clear that a complete description of the modes, and the determination of the corresponding frequencies is, in general, not possible unless one has a knowledge of the nature of the interatomic forces in the crystal lattice. But even in the absence of such information, the symmetry of the lattice brings about a reduction in the number of discrete modes. Thus, if the application of a symmetry operation pertaining to the lattice brings one mode into coincidence with another, then the two must have identical frequencies. Since it is only the *direction* of the axes along which α, β and γ have the prescribed values that is important, one can dispense with the translation group of the space-lattice altogether, and consider only the point-group that is located at each of the lattice points. The only symmetry operators that need be considered are those that belong to this point-group, which is a sub-group of the space-group. Hereafter, by the word " operator " will only be meant a symmetry-operator of the point-group.

The description of a normal mode by the conditions $\alpha = \pm 1$, $\beta = \pm 1$, $\gamma = \pm 1$ shows that there are eight possible types of motion in the most general case, with $3p$ degrees of freedom for each, if there are p atoms in the unit cell. Of these $24p$ degrees of freedom, 3 will represent the translation of the lattice as a whole along three directions, and the remainder $(24p - 3)$ will be the number of vibrational degrees of freedom. In the present case, p is equal to unity, and the number of distinct modes of vibration will be 21 in the general case of a lattice with no symmetry. But if the lattice has some special symmetries, then it is found that the eight types are not distinct, and that some of them may be identical. Thus, they can be classified into a lesser number of sets, where the types in any set give identical frequencies.

The directions of vibration of the three modes in each type can be found as follows. Suppose that the atoms are vibrating in a particular mode. Out of the point-group of operations which brings the lattice into self-coincidence, choose one which brings atoms of the same phase into coincidence, *for that mode.* Then, the mode of vibration after applying this symmetry operation must be the same as the one before. Hence, the directions of vibration in the two cases must either be the *same* or *equivalent.* This must be true for the whole group of symmetry-operations which brings atoms of the same phase into self-coincidence. This group of operations, which may be called the group of that type of vibration, either leaves the directions of vibration invariant, or brings them into one another. We may therefore take the following as a working rule for obtaining all the information about the directions of motion that is possible by using only considerations of symmetry:

For each type of motion, involving a particular combination of α, β, γ, determine all the symmetry operations which bring atoms of the same phase into self-coincidence. With a postulated set of directions for the vibration, find if the directions are left invariant, or brought into one another. In the former case, the vibrations are non-degenerate, but if one direction is brought into another, the vibrations in these directions have the same frequency, and if all the directions are interchanged, the vibration is triply degenerate. If, on the other hand, none of the above possibilities occurs, and a direction is brought into none of the three postulated ones, then it cannot be a direction of motion for the normal mode. Another set of directions is then postulated, and the method is repeated. In this way, not only are the directions of motion determined, but the degeneracies for the vibrations in the type are also known.

For the sake of convenient reference, we shall tabulate the directions of motion and their degeneracies when the group of the type of vibration is one of certain point-groups which will be needed in this paper. The point-groups that come in are all those of the holohedry in each system. The results tabulated here could also be checked by making use of rigorous group-theoretical methods. In the second column are shown the states to which the vibrations belong, and the number of modes coupled in each. These have been arrived at by the standard method of using character tables.

Point-group	States of the vibrations	Description of the directions of vibration
C_i ..	3 coupled in A_u	Three directions unspecifiable.
C_{2h} ..	1 in A_u and 2 coupled in B_g	One direction along the 2-fold axis, and the other two undetermined, lying in the plane perpendicular to it.
D_{2h} or V_h ..	1 in B_{1u}, 1 in B_{2u}, and 1 in B_{3u}	The three directions are orthogonal, and are along the directions of the three 2-fold axes.
D_{4h}	1 in A_{2u} and 1 in E_u	One direction along the 4-fold axis, and the other two degenerate in the perpendicular plane.
D_{3d} ..	1 in A_{2u} and 1 in E_u	One direction along the 3-fold axis, and the other two degenerate in the perpendicular plane.
D_{6h} ..	1 in A_{2u} and 1 in E_{1u}	One direction along the 6-fold axis, and the other two degenerate in the perpendicular plane.
O_h ..	1 in T_{1u}	The vibration is triply degenerate.

Using the above general methods, the modes of vibration will now be worked out for the fourteen Bravais lattices. The primitive translations will

be represented by OA, OB and OC, and α, β, γ will respectively pertain to these three directions.

1. *Triclinic Lattice* Γ_{tr}

This lattice has the highest symmetry of the triclinic system, *i.e.*, that of triclinic holohedry, C_i. The symmetry operations are identity 1 and inversion I. The latter only reverses the direction of the primitive translations, which however does not alter the value of α, β or γ. Hence, no two modes are identical, and there are 21 distinct modes of vibration falling into 7 types. These types can be described as the vibration of atoms in alternate crystallographic planes with opposite phases. Each has three degrees of freedom, but the direction of vibration for these cannot be specified from considerations of symmetry alone, for the group of every one of the eight types is C_i, which brings any direction into self-coincidence. The description of the modes is given below:

No.	α	β	γ	*Description*	*Number of modes*
1 to 3	+	+	+	Translation of the lattice as a whole	1, 1, 1
4 to 6	+	+	−	Vibration of atoms in alternate (001) planes with opposite phases along three unspecified directions ..	1, 1, 1
7 to 9	+	−	+	Same as (4) to (6), but of alternate (010) planes ..	1, 1, 1
10 to 12	−	+	+	Same as (4) to (6), but of alternate (100) planes ..	1, 1, 1
13 to 15	−	−	+	Same as (4) to (6), but of alternate (110) planes ..	1, 1, 1
16 to 18	−	+	−	Same as (4) to (6), but of alternate (101) planes ..	1, 1, 1
19 to 21	+	−	−	Same as (4) to (6), but of alternate (011) planes ..	1, 1, 1
21 to 24	−	−	−	Same as (4) to (6), but of alternate (111) planes ..	1, 1, 1
				Total ..	24

Number of discrete modes of vibration **21.**

2. *Simple Monoclinic Lattice* Γ_m

This has the highest symmetry of the monoclinic system, namely that of the point-group C_{2h}. The symmetry operators are the identity 1, $A(\pi)$, S_h and $A(\pi)\,S_h$, where $A(\pi)$ denotes a 2-fold axis along the z-axis, and S_h a horizontal reflection plane normal to it, containing the x and y axes. Two of the primitive translations OA and OB are taken in the symmetry plane along Ox and Oy respectively, and the third OC is taken perpendicular to them along Oz. Obviously, the application of every one of the symmetry operations only brings the axes into self-coincidence, or reverses their direction, neither of which alters the value of α, β or γ. Hence, here also, we have 21 distinct modes of vibration, but the directions of some of these can be specified. The group of every one of these is verified to be C_{2h}, so

that one direction is along the 2-fold axis Oz, and the other two lie in the plane xOy.

No.	α	β	γ	*Description*	*Number of modes*
1 to 3	+	+	+	Translation of the lattice as a whole	1, 1, 1
4	+	+	−	Vibration of atoms in alternate (001) planes with opposite phases, normally to the planes	1
5, 6	+	+	−	Same as (4), but transversely in two undetermined directions in the plane	1, 1
7 to 9	+	−	+	Vibration of atoms in alternate (010) planes along three directions, one parallel to Oz and the other two in the plane xOy	1, 1, 1
10 to 12	−	+	+	Same as (7) to (9), but of (100) planes	1, 1, 1
13 to 15	−	−	+	Same as (7) to (9), but of (110) planes	1, 1, 1
16 to 18	−	+	−	Same as (7) to (9), but of (101) planes	1, 1, 1
19 to 21	+	−	−	Same as (7) to (9), but of (011) planes	1, 1, 1
22 to 24	−	−	−	Same as (7) to (9), but of (111) planes	1, 1, 1
				Total ..	24

Number of distinct modes of vibration **21.**

3. *Side-Centred Monoclinic Lattice* Γ_m'

In this lattice two opposite sides have atoms at the centre in addition to Γ_m. The primitive translations, as also the directions of the crystallographic axes are marked out in Fig. 1. This lattice has also the point-group symmetry of C_{2h}, and the application of the symmetry operations results in the following:

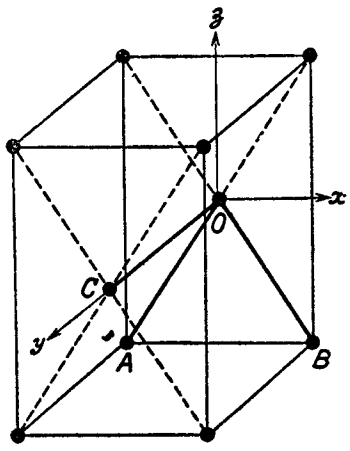

FIG. 1. Side-centred Monoclinic Lattice

1 leaves the primitive translations unaltered, and if we denote the new values of α, β, γ, by α', β', γ', respectively, then $\alpha' = \alpha$, $\beta' = \beta$, $\gamma' = \gamma$.

S_h converts OA$\rightarrow -$ OB, and OB$\rightarrow -$ OA, leaving OC unaltered. Hence, $\beta' = \alpha$, $\alpha' = \beta$, $\gamma' = \gamma$.

A (π) has the same effect on α, β, γ as S_h, and A (π) S_h produces no changes in α, β, γ.

If we work out the effect of these transformations on the eight combinations of α, β and γ, then it is found that + − + and − + + are equivalent, and that so are

$+ - -$ and $- + -$, the rest being distinct. The group of these four is only C_i so that the directions of vibration cannot be specified. For the rest, the group of the vibration is C_{2h}, and one direction is along Oz, the other two lying in xOy. The modes of vibration can, therefore, be described as follows:

No.	α β γ	*Description*	*Number of modes*
1 to 3	$+ + +$	Translation of the lattice as a whole	1, 1, 1
4 to 6	$+ + -$	Vibration of the atoms in alternate (010) planes in three directions, one along Oz, and the other two in the plane xOy	1, 1, 1
7 to 9	$- - +$	Same as (4) to (6), but of (100) planes	1, 1, 1
10 to 12	$+ - +$ / $- + +$	Vibration of atoms in alternate (10$\bar{1}$) and (101) planes with opposite phases in three undetermined directions	2, 2, 2
13 to 15	$+ - -$ / $- + -$	Same as (10) to (12), but of (11$\bar{1}$) and (111) planes ..	2, 2, 2
16 to 18	$- - -$	Same as (4) to (6), but of (011) planes	1, 1, 1
		Total ..	24

Number of distinct modes **15.**

4. Simple Orthorhombic Lattice Γ_o

This lattice has the full symmetry of the orthorhombic system, *i.e.*, of the point-group V_h or D_{2h}. The symmetry operations are 1, U, V, W; S_h, US_h, VS_h, WS_h, where U, V, W are respectively rotations through π about 2-fold axes along Ox, Oy, Oz, and S_h is a reflection on the xy plane. The primitive translations may be taken along Ox, Oy and Oz, so that none of the symmetry operations alters the value of α, β or γ. Thus, for this lattice also, there are 21 modes of vibration, but the directions of the vibration can be specified for all of them, since the group of all the eight types of vibration is D_{2h}.

No.	α β γ	*Description*	*Number of modes*
1 to 3	$+ + +$	Translation of the lattice as a whole	1, 1, 1
4 to 6	$+ + -$	Vibrations of atoms in alternate (001) planes with opposite phases along the directions Ox, Oy, Oz ..	1, 1, 1
7 to 9	$+ - +$	Same as (4) to (6), but of (010) planes	1, 1, 1
10 to 12	$- + +$	Same as (4) to (6), but of (100) planes	1, 1, 1
13 to 15	$- - +$	Same as (4) to (6), but of (110) planes	1, 1, 1
16 to 18	$- + -$	Same as (4) to (6), but of (101) planes	1, 1, 1
19 to 21	$+ - -$	Same as (4) to (6), but of (011) planes	1, 1, 1
22 to 24	$- - -$	Same as (4) to (6), but of (111) planes	1, 1, 1
		Total ..	24

Number of distinct modes **21.**

5. *Side-Centred Orthorhombic Lattice* Γ_0'

This lattice has, in addition to the simple orthorhombic lattice, two points at the centres of two opposite sides. The unit cell of the lattice is shown in Fig. 2, where OA, OB, OC are the primitive translations, and Ox, Oy, Oz are the orthorhombic axes. This lattice also has the pointgroup symmetry of V_h, and the application of the symmetry operations produces the following transformations:

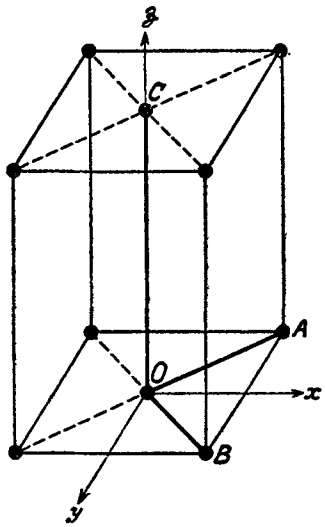

FIG. 2. Side-centred Orthorhombic Lattice

1 leaves α, β, γ unaltered.

U makes $\alpha' = \beta$, $\beta' = \alpha$, $\gamma' = \gamma$.

V makes $\alpha' = \beta$, $\beta' = \alpha$, $\gamma' = \gamma$.

W leaves α, β, γ unaltered, and S_h also does the same, so that S_h U, S_h V, S_h W have the same effect as U, V, W respectively.

Hence, out of the eight combinations of α, β and γ, only 6 are distinct, two pairs being equivalent, *viz.*, $(+\ -\ +,\ -\ +\ +)$; $(+\ -\ -,\ -\ +\ -)$. For these four types, the group is C_{2h}, while for the rest it is V_h. The modes of vibration can, therefore, be described as below :

No.	α	β	γ	*Description*	*Number of modes*
1 to 3	+	+	+	Translation of the lattice as a whole	1, 1, 1
4 to 6	+	+	−	Vibration of atoms in alternate (001) planes with opposite phases along the directions Ox, Oy, Oz ..	1, 1, 1
7 to 9	−	−	+	Same as (4) to (6), but of (100) planes	1, 1, 1
10 to 12	−	−	−	Same as (4) to (6), but of (101) planes	1, 1, 1
13 to 15	+	−	+	Vibration of atoms in alternate (110) and ($1\bar{1}0$) planes along three directions, one along Oz, and the other two in the plane xOy	2, 2, 2
	−	+	+		
16 to 18	+	−	−	Same as (13) to (15), but of ($1\bar{1}1$) and (111) planes..	2, 2, 2
	−	+	−		
				Total ..	24

Number of distinct modes of vibration **15.**

6. *Body-Centred Orthorhombic Lattice* Γ_0'''

This lattice has, in addition to the simple lattice Γ_0, a point at the centre of its unit cell. The primitive translations can be taken as the line joining the centre O to three of the corners A, B, C as shown in Fig. 3. The ortho-

rhombic axes Ox, Oy, Oz will be parallel to the sides of the rectangular parallelepiped. The translation along the fourth direction OD to the adjacent atom may be represented by $(\overrightarrow{OA} + \overrightarrow{OB} + \overrightarrow{OC})$, and the phase change for the translation will be the product of those for OA, OB and OC, *i.e.*, equal to $\alpha\beta\gamma$. This lattice has also the symmetry of the point-group V_h, and the application of the symmetry operations of this group results in the following:

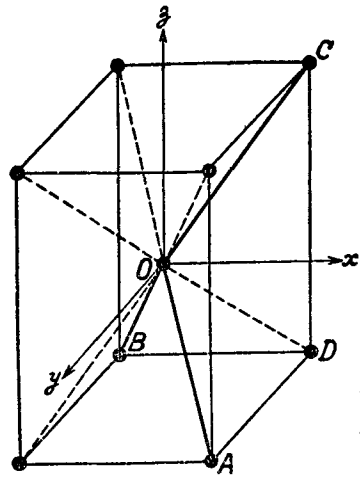

FIG. 3. Body-centred Orthorhombic Lattice

1 leaves α, β, γ unaltered.
U makes $\alpha' = \gamma$, $\beta' = \alpha\beta\gamma$, $\gamma' = \alpha$.
V makes $\alpha' = \alpha\beta\gamma$, $\beta' = \gamma$, $\gamma' = \beta$.
W makes $\alpha' = \beta$, $\beta' = \alpha$, $\gamma' = \alpha\beta\gamma$.
S_h makes $\alpha' = \beta$, $\beta' = \alpha$, $\gamma' = \alpha\beta\gamma$.
S_hU makes $\alpha' = \alpha\beta\gamma$, $\beta' = \gamma$, $\gamma' = \beta$.
S_hV makes $\alpha' = \gamma$, $\beta' = \alpha\beta\gamma$, $\gamma' = \alpha$.
S_hW makes $\alpha' = \alpha$, $\beta' = \beta$, $\gamma' = \gamma$.

On working out the effect of these transformations on the eight combinations of α, β and γ, the following sets become identical: $(+\,+\,-,\ -\,-\,+)$; $(+\,-\,+,\ -\,+\,-)$; $(+\,-\,-,\ -\,+\,+)$. For these six types, the group of the vibration is only C_{2h}, while for $(+\,+\,+)$ and $(-\,-\,-)$, it is V_h. Hence, the modes of vibration are the following:

No.	α	β	γ	*Description*	*Number of modes*
1 to 3	+	+	+	Translation of the lattice as a whole	1, 1, 1
4 to 6	−	−	−	Vibration of the two lattices, composed of the atoms at the centre, and of atoms at the corners, against one another with opposite phase, parallel to Ox, Oy and Oz	1, 1, 1
7 to 9	+	+	−	Vibration of atoms in alternate (110) and (1$\bar{1}$0) planes	
	−	−	+	along three directions, one parallel to Oz, and the other two lying in the plane xOy	2, 2, 2
10 to 12	+	−	+	Same as (7) to (9), but of (011) and (01$\bar{1}$) planes along	
	−	+	−	Ox and two other directions in yOz	2, 2. 2
13 to 15	+	−	−	Same as (7) to (9), but of (101) and (10$\bar{1}$) planes along	
	−	+	+	Oy and two other directions in zOx	2, 2, 2
				Total ..	24

Number of distinct modes **12.**

7. *Face-Centred Orthorhombic Lattice* Γ_0''

This lattice has, in addition to the simple orthorhombic lattice, atoms at the centres of the six faces. The primitive translations OA, OB, OC can be taken as the lines joining a corner to the centres of three faces intersecting at that corner, as shown in Fig. 4. The translations to the centres of the other three sides will be $(\vec{OB} - \vec{OC})$, $(\vec{OC} - \vec{OA})$ and $(\vec{OA} - \vec{OB})$, and the phase changes for these translations are $\beta\gamma$, $\gamma\alpha$ and $\alpha\beta$ respectively. Applying the symmetry operations of the point-group V_h, to which the lattice belongs, to the eight combinations of α, β, γ, we find that

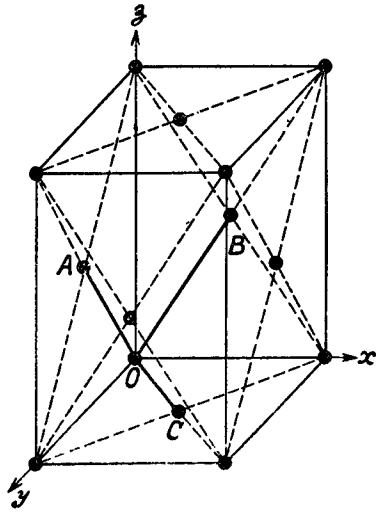

FIG. 4. Face-centred Orthorhombic Lattice

1 leaves α, β, γ unaltered.
U makes $\alpha' = \alpha$, $\beta' = \gamma\alpha$, $\gamma' = \alpha\beta$.
V makes $\alpha' = \beta\gamma$, $\beta' = \beta$, $\gamma' = \alpha\beta$.
W makes $\alpha' = \beta\gamma$, $\beta' = \gamma\alpha$, $\gamma' = \gamma$.
S_h makes $\alpha' = \beta\gamma$, $\beta' = \gamma\alpha$, $\gamma' = \gamma$.
S_hU makes $\alpha' = \beta\gamma$, $\beta' = \beta$, $\gamma' = \alpha\beta$.
S_hV makes $\alpha' = \alpha$, $\beta' = \gamma\alpha$, $\gamma' = \alpha\beta$
S_hW makes $\alpha' = \alpha$, $\beta' = \beta$, $\gamma' = \gamma$.

Working out these transformations, the following become equivalent (+ + −, + − +, − + +, − − −), and the other four are left invariant. The group of the vibration in this set of four is only C_i, so that the directions cannot be specified. For the rest, the group is V_h, and the vibrations take place along Ox, Oy, Oz. The modes of vibration can be described as below:

No.	α	β	γ	*Description*	*Number of modes*
1 to 3	+	+	+	Translation of the lattice as a whole	1, 1, 1
4 to 6	+	−	−	Vibration of atoms in alternate (100) planes along Ox, Oy, Oz with opposite phases	1, 1, 1
7 to 9	−	+	−	Same as (4) to (6), but of (010) planes	1, 1, 1
10 to 12	−	−	+	Same as (4) to (6), but of (001) planes	1, 1, 1
13 to 15	+	+	−	Vibrations of atoms in alternate (111), (1$\bar{1}$1), (11$\bar{1}$),	
	+	−	+	($\bar{1}$11) planes in three unspecifiable directions ..	4, 4, 4
	−	+	+		
	−	−	−		
				Total ..	24

Total number of distinct modes **12**.

8. *Simple Tetragonal Lattice* Γ_t

This lattice possesses the full symmetry of the tetragonal system, *i.e.*, of the point-group D_{4h}. The symmetry-operations are 1, A$(\pi/2)$, A(π), A$(3\pi/2)$; U, A$(\pi/2)$U, A(π)U, A$(3\pi/2)$U; S_h, A$(\pi/2)S_h$, A$(\pi)S_h$, A$(3\pi/2)S_h$; US_h, A$(\pi/2)US_h$, A$(\pi)US_h$, A$(3\pi/2)US_h$. Here, A is a four-fold axis along Oz, and U represents a rotation through π about a twofold axis along Ox. S_h denotes a reflection in the plane xOy. We take the primitive translations along Ox, Oy, Oz respectively. Then, the application of U, A(π) and S_h does not alter the values of α, β, γ; but the operations A$(\pi/2)$ and A$(3\pi/2)$ bring about an interchange of α and β, $\alpha \leftrightarrows \beta$, leaving γ unaltered. Hence, out of the eight combinations of α, β, γ, two become equivalent with two others, *viz.*, $(+\ -\ +,\ -\ +\ +)$; $(+\ -\ -,\ -\ +\ -)$, and there are only six distinct sets. For the four types, $+\ -\ +$, $-\ +\ +$, $+\ -\ -$ and $-\ +\ -$, the group of the vibration is V_h, and the directions of vibration are distinct and lie along Ox, Oy, Oz. For the other four, the group is D_{4h}, so that one vibration is along Oz, and the other two are degenerate in the plane xOy. The modes of vibration may therefore be described as follows:

No.	α β γ	*Description*	*Number of modes*
1, 2	+ + +	Translation of the lattice as a whole	1, 2
3	+ + −	Vibration of alternate basal (001) planes normally along Oz, with opposite phases	1
4	+ + −	Same as (3), but transversely along Ox and Oy, which are, however, degenerate	2
5	+ − +	Vibration of alternate prismatic (100) and (010) planes	
	− + +	normally	2
6	+ − +	Same as (5), but transversely parallel to the tetragonal	
	− + +	axis Oz	2
7	+ − +	Same as (5), but transversely along the third perpendi-	
	− + +	cular direction, *i.e.*, Oy and Ox respectively ..	2
8	+ − −	Vibration of atoms in alternate (101), (011) planes	
	− + −	along Oz, with opposite phase	2
9, 10	+ − −	Same as (8), but along Ox and Oy	2, 2
	− + −		
11	− + −	Vibration of atoms in alternate (110) planes along the 4-fold axis Oz	1
12	− − +	Same as (11), but in two directions in the plane xOy, which are degenerate	2
13	− − −	Same as (11), but of (111) planes along Oz	1
14	− − −	Same as (11), but of (111) planes along two directions in xOy, which are degenerate	2
		Total ..	24

Number of distinct modes of vibration **12.**

9. *Body-Centred Tetragonal Lattice* Γ_t'

This lattice has, in addition to the simple lattice Γ_t, an atom at the centre of the square prism, and has the symmetry of the point-group D_{4h}. The primitive translations can be taken, as in the body-centred orthorhombic lattice, to lie along the lines joining the centre to three of the corners. In fact, Fig. 3 will suffice for this lattice, but it must be remembered that Oz is a four-fold axis in this case, and that Ox and Oy are equivalent. The effect of the symmetry operations on the primitive translations is as follows:

1 leaves α, β, γ unaltered.

A $(\pi/2)$	makes $\alpha' = \gamma$,	$\beta' = \alpha\beta\gamma$,	$\gamma' = \beta$.
A (π)	makes $\alpha' = \beta$,	$\beta' = \alpha$,	$\gamma' = \alpha\beta\gamma$.
A $(3\pi/2)$	makes $\alpha' = \alpha\beta\gamma$,	$\beta' = \gamma$,	$\gamma' = \alpha$.
U	makes $\alpha' = \gamma$,	$\beta' = \alpha\beta\gamma$,	$\gamma' = \alpha$.
A $(\pi/2)$ U	makes $\alpha' = \alpha$,	$\beta' = \beta$,	$\gamma' = \alpha\beta\gamma$.
A (π) U	makes $\alpha' = \alpha\beta\gamma$,	$\beta' = \gamma$,	$\gamma' = \beta$.
A $(3\pi/2)$ U	makes $\alpha' = \beta$,	$\beta' = \alpha$,	$\gamma' = \gamma$.
S_h	makes $\alpha' = \beta$,	$\beta' = \alpha$,	$\gamma' = \alpha\beta\gamma$.
A $(\pi/2)$ S_h	makes $\alpha' = \alpha\beta\gamma$,	$\beta' = \gamma$,	$\gamma' = \alpha$.
A (π) S_h	makes $\alpha' = \alpha$,	$\beta' = \beta$,	$\gamma' = \gamma$.
A $(3\pi/2)$ S_h	makes $\alpha' = \gamma$,	$\beta' = \alpha\beta\gamma$,	$\gamma' = \beta$.
US_h	makes $\alpha' = \alpha\beta\gamma$,	$\beta' = \gamma$,	$\gamma' = \beta$.
A $(\pi/2)$ US_h	makes $\alpha' = \beta$,	$\beta' = \alpha$,	$\gamma' = \gamma$.
A (π) US_h	makes $\alpha' = \gamma$,	$\beta' = \alpha\beta\gamma$,	$\gamma' = \alpha$.
A $(3\pi/2)$ US_h	makes $\alpha' = \alpha$,	$\beta' = \beta$,	$\gamma' = \alpha\beta\gamma$.

Using these, one finds that there are only four distinct sets, the following being equivalent $(+\ +\ -,\ -\ -\ +)$; $(+\ -\ -,\ -\ +\ +,\ +\ -\ +,\ -\ +\ -)$. Of these, only $(+\ +\ +)$ and $(-\ -\ -)$ have D_{4h} as the group of their vibration. The group of $(+\ +\ -)$ and $(-\ -\ +)$ is V_h, and of the rest, C_{2h}. Hence, the modes of vibration are as follows:

No.	α	β	γ	*Description*	*Number of modes*
1, 2	+	+	+	Translation of the lattice as a whole	1, 2
3	+	+	−	Vibration of atoms in alternate (110), $(1\bar{1}0)$ planes	
	−	−	+	normally, with opposite phase	2
4	+	+	−	Same as (3), but transversely along the tetragonal	
	−	−	+	axis, Oz	2
5	+	+	−	Same as (3), but transversely perpendicular to Oz ..	2
	−	−	+		

No.	$\alpha\ \beta\ \gamma$	*Description*	*Number of modes*
6 to 8	$+\ -\ -$ $-\ +\ +$ $+\ -\ +$ $-\ +\ -$	Vibration of atoms in alternate (011), (01$\bar{1}$) planes along Ox, and two other directions in yOz, and of (101), (10$\bar{1}$) planes along Oy and two other directions in zOx	4, 4, 4
9	$-\ -\ -$	Oscillation of the two lattices composed of the atoms at the centre, and those at the corners, against one another, along Oz	1
10	$-\ -\ -$	Same as (9), but along two directions in xOy, which are degenerate	2
		Total ..	24

Number of distinct modes of vibration **8**.

10. Rhombohedral Bravais Lattice Γ_{rh}

This lattice has the full symmetry of the rhombohedral division of the hexagonal system, *i.e.*, of the point-group D_{3d}. The unit cell and the primitive translations are shown in Fig. 5, where Ox, Oy, Oz are the hexagonal crystallographic axes. The symmetry operations of the point-group D_{3d} are

1, A$(2\pi/3)$, A$(4\pi/3)$; U, A$(2\pi/3)$ U, A$(4\pi/3)$ U;
I, A$(2\pi/3)$ I, A$(4\pi/3)$ I; UI, A$(2\pi/3)$ UI, A$(4\pi/3)$ UI.

Here, A is a threefold rotation axis along 0z, U is a twofold axis along Ox, and I is the operation of inversion. Of these,

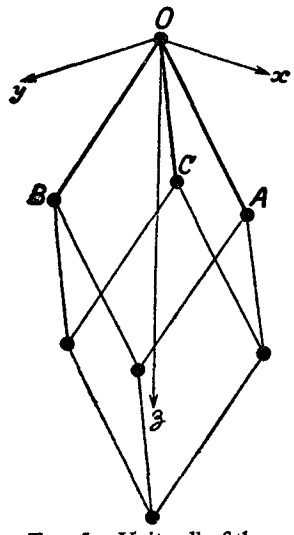

FIG. 5. Unit cell of the Rhombohedral Lattice

A$(2\pi/3)$ makes $\alpha' = \beta,\ \beta' = \gamma,\ \gamma' = \alpha$.
A$(4\pi/3)$ makes $\alpha' = \gamma,\ \beta' = \alpha,\ \gamma' = \beta$.
U makes $\alpha' = \alpha,\ \beta' = \gamma,\ \gamma' = \beta$.
A$(2\pi/3)$ U makes $\alpha' = \gamma,\ \beta' = \beta,\ \gamma' = \alpha$.
A$(4\pi/3)$ U makes $\alpha' = \beta,\ \beta' = \alpha,\ \gamma' = \gamma$.

I leaves α, β, γ unaltered, so that the other operations produce only similar transformations.

Applying these to the eight combinations of α, β, γ, one finds that they split up into four sets, $(+\ +\ +)$; $(-\ -\ -)$; $(+\ +\ -,\ +\ -\ +,\ -\ +\ +)$; $(-\ -\ +,\ -\ +\ -,\ +\ -\ -)$. The group of the first two sets is D_{3d}, but for the types of vibration in the other two, the group is only C_{2h}, so that the vibration is specifiable in only one direction, the other two lying in a perpendicular plane. The modes of vibration may therefore be described as follows, using rhombohedral indices.

No.	α β γ	*Description*	*Number of modes*
1, 2	+ + +	Translation of the lattice as a whole	1, 2
3	− − −	Vibration of alternate (111) planes normally along the 3-fold axis, Oz	1
4	− − −	Same as (3), but transversely, the vibration being degenerate in the plane..	2
5	− − +	Vibration of atoms in alternate $(1\bar{1}0)$, $(10\bar{1})$, $(01\bar{1})$	
	− + −	planes along the normal to the plane	3
	+ − −		
6, 7	− − +	Same as (5), but transversely in two directions in the	
	− + −	plane	3, 3
	+ − −		
8 to 10	+ + −	Same as (5) to (7), but of atoms in alternate (001),	
	+ − +	(010), (100) planes, which form the sides of the	
	− + +	rhombohedral unit cell	3, 3, 3
		Total ..	24

Number of distinct modes **8.**

11. Hexagonal Bravais Lattice Γ_h

This lattice, which is shown in Fig. 6, has the full symmetry of the hexagonal system, *i.e.*, of the point-group D_{6h}. The symmetry operations are $\{C_6\} \equiv 1$, A $(\pi/3)$, A $(2\pi/3)$, A (π), A $(4\pi/3)$, A $(5\pi/3)$, where C_6 is a sixfold axis parallel to $0z$, $\{C_6U\}$, where U is a twofold axis along Ox, $\{C_6S_h\}$ and $\{C_6US_h\}$, where S_h denotes reflection in the plane xOy. The primitive translations OA, OB, OC lie in this case along the hexagonal axes Ox, Oy, Oz respectively. The effect of symmetry operations on α, β, γ is easily seen to be as below:

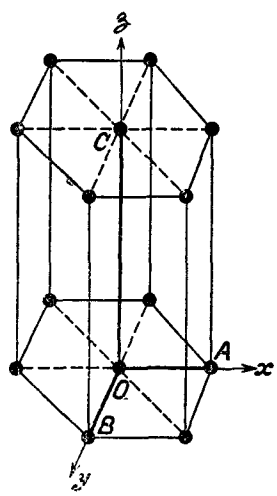

FIG. 6. Hexagonal Bravais Lattice

1 leaves α, β, γ unaltered.

A $(\pi/3)$, A $(4\pi/3)$ make $\alpha' = \alpha\beta$, $\beta' = \alpha$, $\gamma' = \gamma$.

A $(2\pi/3)$, A $(5\pi/3)$ make $\alpha' = \beta$, $\beta' = \alpha\beta$, $\gamma' = \gamma$.

A (π) makes $\alpha' = \alpha$, $\beta' = \beta$, $\gamma' = \gamma$.

U makes $\alpha' = \alpha$, $\beta' = \alpha\beta$, $\gamma' = \gamma$.

A $(\pi/3)$ U, A $(4\pi/3)$ U make $\alpha' = \beta$, $\beta' = \alpha$, $\gamma' = \gamma$.

A $(2\pi/3)$ U, A $(5\pi/3)$ U make $\alpha' = \alpha\beta$, $\beta' = \beta$, $\gamma' = \gamma$.

S_h leaves α, β, γ unaltered, so that the others need not be considered.

The combinations of α, β, γ thus reduce to the four sets (+ + +); (+ + −); (+ − −, − + −, − − −); (− − +, + − +, − + +).

For the first two types, the group of the vibration is D_{6h}, and for the others it is only V_h. The modes of vibration are, therefore,

No.	α	β	γ	*Description*	*Number of modes*
1, 2	+	+	+	Translation of the lattice as a whole	1, 2
3	+	+	−	Vibration of alternate (0001) basal planes against one another normally, along $0z$	1
4	+	+	−	Same as (3), but transversely, degenerate in the plane ..	2
5	−	−	+	Vibration of atoms in alternate prismatic planes $(01\bar{1}0)$,	
	+	−	+	$(10\bar{1}0)$, $(1\bar{1}00)$ with opposite phases, normally to	
	−	+	+	the plane	3
6	−	−	+	Same as (5), but transversely along the hexagonal	
	+	−	+	axis Oz	3
	−	+	−		
7	−	−	+	Same as (5), but transversely perpendicular to Oz ..	3
	+	−	+		
	−	+	+		
8 to 10	−	−	−	Same as (5) to (7), but of the planes $(01\bar{1}1)$, $(10\bar{1}1)$,	
	+	−	−	$(1\bar{1}01)$ planes along the same directions as in (5)	
	−	+	−	to (7)	3, 3, 3
				Total ..	24

Total number of distinct modes **8.**

12. Simple Cubic Lattice Γ_c

This, and the next two lattices have been discussed by E. V. Chelam in another paper appearing in this symposium. However, for the sake of completeness, and for a clearer understanding of the methods proposed in this paper, they are also tabulated. The full symmetry operations, and the detailed working will not be given here.

The simple cubic lattice has the highest symmetry of the cubic system, *i.e.*, of the point-group O_h. Taking the primitive translations along the cube axes, an application of the symmetry operations shows that the eight combinations of α, β, γ fall into four sets, $(+\ +\ +)$; $(-\ -\ -)$; $(+\ +\ -,\ +\ -\ +,\ -\ +\ +)$; $(-\ -\ +,\ -\ +\ -,\ +\ -\ -)$. Of these, the group of the vibrations of the type $(+\ +\ +)$ and $(-\ -\ -)$ is 0_h, so that they are triply degenerate. The group of the remaining six is D_{4h}. The modes of vibration may therefore be described as follows:

No.	α β γ	*Description*	*Number of modes*
1	+ + +	Translation of the lattice as a whole	3
2	− − −	Vibrations of alternate octahedral (111) planes with opposite phase, triply degenerate	3
3	+ + −	Vibration of alternate cube faces with opposite phase,	
	+ − +	normally	3
	− + +		
4	+ + −	Same as (3), but transversely, the vibration being	
	+ − +	degenerate in the plane	6
	− + +		
5	− − +	Vibration of atoms in alternate dodecahedral {110}	
	− + −	planes with opposite phase along the cube axis in	
	+ − −	the plane	3
6	− − +	Same as (5), but along the normal to the plane, and	
	− + −	along the third orthogonal direction, *i.e.*, the dodeca-	
	+ − −	hedral axis in the plane, the two being of the same	
		frequency	6
		Total ..	24

Number of distinct modes **5**.

13. Face-Centred Cubic Lattice Γ_c'

This lattice has points at the centres of the six cube faces in addition to those at the corners. The primitive translations may be taken as the lines joining a corner to the points at the centre of any three faces intersecting at that corner. Applying the symmetry operations of the point-group O_h to which this lattice belongs, the eight possible combinations of α, β, γ fall into three sets, (+ + +); (+ + −, + − +, − + +, − − −); (− − +, − + −, + − −). The group for the vibration in the first set is O_h, that for the second set is D_{3d} and for the third D_{4h}. The vibration in the first set is therefore triply degenerate, and in the other two, one vibration is along the threefold or fourfold axis, and two vibrations are degenerate in the perpendicular plane. The modes of vibration are as follow:

No.	α β γ	*Description*	*Number of modes*
1	+ + +	Translation of the lattice as a whole	3
2	+ − +	Vibration of alternate {111} octahedral planes with	
	+ − +	opposite phases, normally	4
	− + −		
	− − −		

No.	α β γ	*Description*	*Number of modes*
3	+ + − + − + − + + − − −	Same as (2), but transversely degenerate in the plane..	8
4	− − + − + − + − −	Vibrations of alternate {100} cube faces normally ..	3
5	− − + − + − + − −	Same as (6), but transversely the vibration being degenerate in the plane	6
		Total ..	24

Number of distinct modes **4**.

14. Body-Centred Cubic Lattice Γ_c''

This lattice has a point at the centre of the cube in addition to Γ_c, and possesses the symmetry of O_h. The primitive translations may be taken along the lines joining the centre to any three of the cube corners. An application of the symmetry operations shows that there are only three sets of combinations of α, β, γ, *viz.*, (+ + +); (− − −); (+ + −, + − +, − + +, − − +, − + −, + − −). Except the first two, whose group is O_h, the group of all the other six types of vibration is only V_h, so that the vibrations along the three directions are of different frequencies.

No.	α β γ	*Description*	*Number of modes*
1	+ + +	Translation of the lattice as a whole	3
2	− − −	Triply degenerate vibration of the two interpenetrating cubic lattices against one another	3
3 to 5	+ + − + − + − + + − − + − + − + − −	Vibrations of alternate {110} dodecahedral planes, with opposite phases, in three directions, normally, transversely parallel to a cube axis, and transversely along the dodecahedral axis in the plane ..	6, 6, 6
		Total ..	24

Number of distinct modes **4**.

The work reported in this paper was undertaken at the suggestion of Prof. Sir C. V. Raman to whom I am extremely grateful for the many helpful discussions I had with him.

Summary

In this paper, the degeneracies and the directions of the normal modes of vibration in the fourteen Bravais lattices are worked out from symmetry considerations, making use of Sir C. V. Raman's theory. Denoting the ratio of the displacements of adjacent atoms along the primitive translations by α, β, γ, these can have only the values $+1$ or -1, so that the vibrations fall into eight types in the general case of no symmetry. In lattices possessing symmetry, however, some of the types could be brought over into others by the application of symmetry operations, and thus would be equivalent with the latter. Also, the directions of motion in any particular type of vibration may be equivalent. This is determined by selecting a group of operations which brings the atoms of the same phase to coincide for that type of vibration, and finding the directions of motion which satisfy the symmetry requirements of this group. In this way, both the directions of motion and their degeneracies are known. The number of distinct modes of vibration computed for the various lattices, are for Γ_{tr} 21; Γ_m 21, Γ_m' 15; Γ_0 21, Γ_0' 15, Γ_0'' and Γ_0''' 12; Γ_t 12, Γ_t' 8; Γ_{rh} 8, Γ_h 8; Γ_c5, Γ_c' 4, Γ_c'' 4. The modes are also described in as complete a manner as could be done by using considerations of symmetry alone.