

with these values, because they were derived from prisms of orientations which involve all the four constants, but without taking such a fact into account.

It may be noted that the stress-optical constants for ammonium alum are the largest known of all cubic crystals so far studied.

Four independent constants are required for describing the photo-elastic behaviour in class $T_h-2/m\bar{3}$, because the cube axes are only digonal and not tetragonal. It can now be stated as a general rule applicable to all cubic crystals, that pressure along any axis of trigonal or tetragonal symmetry makes the crystal optically uniaxial, whereas pressure along any digonal axis, or in a general direction, makes the crystal biaxial.

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Note on the Bhagavantam-Suryanarayana Method of Enumerating the Physical Constants of Crystals

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(Received 10 August 1948 and in revised form 5 October 1948)

A method alternative to that of Bhagavantam and Suryanarayana is given for enumerating, by group theory, the number of independent constants for any physical property of crystals in the 32 classes; the method consists of finding first the explicit form of the representation in question for the full group of all rotations and reflexions and then obtaining the form for the individual crystal classes by specialization.

In this journal Bhagavantam & Suryanarayana (1949) have described a group-theoretical method of determining the number of independent constants describing various physical properties of crystals in each of the 32 crystal classes, their method being a variant of a method developed by the present author (Jahn, 1937) in a paper on the enumeration of the elastic constants of crystals. It is the purpose of this note to show that the results of Bhagavantam & Suryanarayana may be obtained in a different manner which adheres more closely to the original method of the writer.

Bhagavantam & Suryanarayana consider a number of different types of physical properties (relations between tensors) for which they list the character of the appropriate representation. It may be verified that the representation in each case is expressible in terms of

that of a polar vector as shown in the accompanying Table I.†

In Table I, V denotes the representation of a polar vector and the notation of Tisza (1933) is used for the symmetrical product, $[V^2]$, of V with itself and higher

† *Notation for irreducible representations.* In this paper, the standard notation used in molecular spectroscopy for the irreducible representations of the symmetry groups is adhered to: thus A or B denote always one-dimensional representations, E two-dimensional, F three-dimensional; different representations being distinguished by different suffixes. The $(2L+1)$ -dimensional representation of the group (R_∞) of all rotations is denoted by D_L . g and u distinguish representations which are even or odd with respect to inversion, whilst a single or a double prime ('') is used to distinguish representations which are even or odd with respect to a plane of symmetry. For a detailed account of this notation, which goes back to Tisza (1933), and for a full account of the algebra of irreducible representations, the reader is referred to the book by Herzberg (1945).

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symmetrical products, e.g. the symmetrical cube $[V^3]$. ϵ denotes the representation of a pseudo scalar: $\epsilon = -1$ if the symmetry operation involves an inversion, $\epsilon = +1$ otherwise.

The number of independent constants describing each property is then given by the number of times the

the extension of this to the symmetrical cube, viz.

$$[(\sum_a D_a)^3] = \sum_a [D_a^3] + \sum_a \sum_{b \neq a} D_a [D_b^2] + \sum_a \sum_{b < c} D_a D_b D_c,$$

which may be proved in the same way, using Tisza's expressions for the characters. (It is easy to verify that $[D_2^3] = D_0 + D_2 + D_3 + D_4 + D_6$.)

Table 1. Enumeration of physical constants for isotropic solids

No.	Representation	R_∞^i	R_∞^i	R_∞^i	Physical property
1	1	D_0^g	1	1	
2	V	D_1^u	0	0	pyro-electricity
3, 3 (a)	$[V^2]$	$D_0^g + D_2^g$	1	1	thermal expansion
4, 5	V^2	$D_0^g + D_1^g + D_2^g$	1	1	
6	$V [V^2]$	$2D_1^u + D_2^u + D_3^u$	0	0	piezo-electricity
7	V^3	$D_0^g + 3D_1^g + 2D_2^g + D_3^g$	0	1	
8 (a)	$[[V^2]^2]$	$2D_0^g + 2D_2^g + D_4^g$	2	2	elasticity
8	$[V^2]^2$	$2D_0^g + D_1^g + 3D_2^g + D_3^g + D_4^g$	2	2	photo-elasticity
9	$V^2 [V^2]$	$2D_0^g + 3D_1^g + 4D_2^g + 2D_3^g + D_4^g$	2	2	
10	V^4	$3D_0^g + 6D_1^g + 6D_2^g + 3D_3^g + D_4^g$	3	3	
11	$V [[V^2]^2]$	$4D_1^u + 2D_2^u + 3D_3^u + D_4^u + D_5^u$	0	0	
12	$[[V^2]^3]$	$3D_0^g + 3D_2^g + D_3^g + 2D_4^g + D_6^g$	3	3	2nd order elasticity
13	$[V^2] [[V^2]^2]$	$4D_0^g + 2D_1^g + 7D_2^g + 3D_3^g + 4D_4^g + D_5^g + D_6^g$	4	4	
E	ϵ	D_0^u	0	1	enantiomorphism
O	$\epsilon [V^2]$	$D_0^u + D_2^u$	0	1	optical activity

Table 2. Enumeration of physical constants for crystals of cubic symmetry

No.	Representation	T_d	O as T_d except as below	30 T_d	28 T	29 T^i	31 O	32 O^i
1	1	A_1		1	1	1	1	1
2	V	F_2	F_1	0	0	0	0	0
3, 3 (a)	$[V^2]$	$A_1 + E + F_2$		1	1	1	1	1
4, 5	V^2	$A_1 + E + F_1 + F_2$		1	1	1	1	1
6	$V [V^2]$	$A_1 + E + 2F_1 + 3F_2$	$A_2 + E + 3F_1 + 2F_2$	1	1	0	0	0
7	V^3	$A_1 + A_2 + 2E + 3F_1 + 4F_2$	$A_1 + A_2 + 2E + 4F_1 + 3F_2$	1	2	0	1	0
8 (a)	$[[V^2]^2]$	$3A_1 + 3E + F_1 + 3F_2$		3	3	3	3	3
8	$[V^2]^2$	$3A_1 + A_2 + 4E + 3F_1 + 5F_2$		3	4	4	3	3
9	$V^2 [V^2]$	$3A_1 + 2A_2 + 5E + 6F_1 + 7F_2$		3	5	5	3	3
10	V^4	$4A_1 + 3A_2 + 7E + 10F_1 + 10F_2$		4	7	7	4	4
11	$V [[V^2]^2]$	$3A_1 + A_2 + 4E + 7F_1 + 10F_2$	$A_1 + 3A_2 + 4E + 10F_1 + 7F_2$	3	4	0	1	0
12	$[[V^2]^3]$	$6A_1 + 2A_2 + 6E + 4F_1 + 8F_2$		6	8	8	6	6
13	$[V^2] [[V^2]^2]$	$9A_1 + 4A_2 + 13E + 12F_1 + 17F_2$		9	13	13	9	9
E	ϵ	A_2	A_1	0	1	0	1	0
O	$\epsilon [V^2]$	$A_2 + E + F_1$	$A_1 + E + F_2$	0	1	0	1	0

identical representation occurs in the reduced form of the appropriate representation, as is shown in Table 1 for the group of all rotations and reflexions R_∞^i (isotropic solid). Bhagavantam & Suryanarayana evaluate this number by a character calculation which for complicated groups is lengthy. The reduced form of the representation, however, may be derived in each case directly and relatively simply using the methods of Tisza and the present writer. Thus the derivation of the results contained in Table 1 required, in addition to the formula already given (Jahn, 1937) for the symmetrical product of a reducible representation, viz.

$$[(\sum_a D_a)^2] = \sum_a [D_a^2] + \sum_{a < b} D_a D_b,$$

Since each of the 32 crystallographic groups is a subgroup of R_∞^i , the number of independent constants can be determined from Table 1 when we know the reduced form of the representations D_L^g, D_L^u for the group in question. These have been listed by the present writer (Jahn, 1938, Table 1) for the group T_d and from these it is easy to derive the results for all the groups of the cubic system as shown in Table 2.

As shown in Table 2, the results for the group O are the same as for the group T_d except for the representations containing odd powers of V or ϵ , for which we must interchange A_1 with A_2 (and F_1 with F_2). The results for T are obtained from T_d by identifying A_1 and A_2 . The number of constants for T^i and O^i is the same as for

T and O except when the representation contains odd powers of V or ϵ , in which case there are no constants.

For the remaining crystallographic groups it is convenient to consider first the axial groups $C_{\infty v}$, D_{∞}^h , D_{∞} . The reduced forms of the representations for these groups are contained in Table 3 and they may be derived from Table 1, using the following reduction of D_L^u , D_L^v for the sub-groups in question:

$$C_{\infty v}: D_L^u = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} + E_1 + E_2 + \dots + E_L \text{ for } L \begin{cases} \text{even} \\ \text{odd} \end{cases},$$

$$D_L^u = \begin{pmatrix} A_2 \\ A_1 \end{pmatrix} + E_1 + E_2 + \dots + E_L \text{ for } L \begin{cases} \text{even} \\ \text{odd} \end{cases}.$$

$$D_{\infty}^h: D_L^u = \begin{pmatrix} A_1' \\ A_2' \end{pmatrix} + E_1'' + E_2'' + E_3'' \dots + \begin{pmatrix} E_L' \\ E_L'' \end{pmatrix} \text{ for } L \begin{cases} \text{even} \\ \text{odd} \end{cases},$$

$$D_L^u = \begin{pmatrix} A_1'' \\ A_2'' \end{pmatrix} + E_1' + E_2' + E_3' \dots + \begin{pmatrix} E_L'' \\ E_L' \end{pmatrix} \text{ for } L \begin{cases} \text{even} \\ \text{odd} \end{cases}.$$

$$D_{\infty}: D_L^u \text{ or } u = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} + E_1 + E_2 + \dots + E_L \text{ for } L \begin{cases} \text{even} \\ \text{odd} \end{cases}.$$

This leads to the same results for D_{∞} as for $C_{\infty v}$ except where the representation contains odd powers of V or ϵ , in which case A_1 and A_2 must be interchanged. For C_{∞}

we obtain the results from $C_{\infty v}$ by putting $A_1 = A_2 = A$. For C_{∞}^h the results follow from D_{∞}^h when we put

$$A_1' = A_2' = A'; \quad A_1'' = A_2'' = A''.$$

From the results contained in Table 3 we can read off the number of constants for the 25 crystallographic groups listed in Table 4, using the following results of Tisza:

(1) For

$$C_{2v} \text{ and } D_2: E_2 = E_4 = E_6 = \dots = E_0 = A_1 + A_2, \\ \text{i.e. } E_2, E_4, E_6 \rightarrow A_1,$$

$$C_{3v} \text{ and } D_3: E_3 = E_6 = \dots = E_0 = A_1 + A_2, \\ \text{i.e. } E_3, E_6 \rightarrow A_1,$$

$$C_{4v} \text{ and } D_4: E_4 = \dots = E_0 = A_1 + A_2, \\ \text{i.e. } E_4 \rightarrow A_1,$$

$$C_{6v} \text{ and } D_6: E_6 = \dots = E_0 = A_1 + A_2, \\ \text{i.e. } E_6 \rightarrow A_1.$$

(2) For C_v , $A_1 = A_2 = A$, so that, for

$$C_2: E_2, E_4, E_6 \rightarrow 2A,$$

$$C_3: E_3, E_6 \rightarrow 2A,$$

$$C_4: E_4 \rightarrow 2A,$$

$$C_6: E_6 \rightarrow 2A.$$

Table 3. Reduction of representations for the full axial groups

No.	Representation	$\begin{cases} C_{\infty v} \\ D_{\infty}^h \end{cases}$	D_{∞} as $C_{\infty v}$, except as below
1	1	$\begin{cases} A_1 \\ A_1' \end{cases}$	
2	V	$\begin{cases} A_1 + E_1 \\ A_2' + E_1' \end{cases}$	$A_2 + E_1$
3, 3 (a)	$[V^2]$	$\begin{cases} 2A_1 + E_1 + E_2 \\ 2A_1' + E_1' + E_2' \end{cases}$	
4, 5	V^2	$\begin{cases} 2A_1 + A_2 + 2E_1 + E_2 \\ 2A_1' + A_2' + 2E_1' + E_2' \end{cases}$	
6	$V[V^2]$	$\begin{cases} 3A_1 + A_2 + 4E_1 + 2E_2 + E_3 \\ A_1' + 3A_2' + 4E_1' + 2E_2' + E_3' \end{cases}$	$A_1 + 3A_2 + 4E_1 + 2E_2 + E_3$
7	V^3	$\begin{cases} 4A_1 + 3A_2 + 6E_1 + 3E_2 + E_3 \\ 3A_1' + 4A_2' + 6E_1' + 3E_2' + E_3' \end{cases}$	$3A_1 + 4A_2 + 6E_1 + 3E_2 + E_3$
8 (a)	$[[V^2]^2]$	$\begin{cases} 5A_1 + 3E_1 + 3E_2 + E_3 + E_4 \\ 5A_1' + 3E_1' + 3E_2' + E_3' + E_4' \end{cases}$	
8	$[V^2]^3$	$\begin{cases} 6A_1 + 2A_2 + 6E_1 + 5E_2 + 2E_3 + E_4 \\ 6A_1' + 2A_2' + 6E_1' + 5E_2' + 2E_3' + E_4' \end{cases}$	
9	$V^2[V^2]$	$\begin{cases} 7A_1 + 5A_2 + 10E_1 + 7E_2 + 3E_3 + E_4 \\ 7A_1' + 5A_2' + 10E_1' + 7E_2' + 3E_3' + E_4' \end{cases}$	
10	V^4	$\begin{cases} 10A_1 + 9A_2 + 16E_1 + 10E_2 + 4E_3 + E_4 \\ 10A_1' + 9A_2' + 16E_1' + 10E_2' + 4E_3' + E_4' \end{cases}$	
11	$V[[V^2]^2]$	$\begin{cases} 8A_1 + 3A_2 + 11E_1 + 7E_2 + 5E_3 + 2E_4 + E_5 \\ 3A_1' + 8A_2' + 11E_1' + 7E_2' + 5E_3' + 2E_4' + E_5' \end{cases}$	$3A_1 + 8A_2 + 11E_1 + 7E_2 + 5E_3 + 2E_4 + E_5$
12	$[[V^2]^3]$	$\begin{cases} 9A_1 + A_2 + 7E_1 + 7E_2 + 4E_3 + 3E_4 + E_5 + E_6 \\ 9A_1' + A_2' + 7E_1' + 7E_2' + 4E_3' + 3E_4' + E_5' + E_6' \end{cases}$	
13	$[V^2][[V^2]^2]$	$\begin{cases} 16A_1 + 6A_2 + 18E_1 + 16E_2 + 9E_3 + 6E_4 + 2E_5 + E_6 \\ 16A_1' + 6A_2' + 18E_1' + 16E_2' + 9E_3' + 6E_4' + 2E_5' + E_6' \end{cases}$	
E	ϵ	$\begin{cases} A_2 \\ A_1' \end{cases}$	A_1
O	$\epsilon[V^2]$	$\begin{cases} 2A_2 + E_1 + E_2 \\ 2A_1' + E_1' + E_2' \end{cases}$	$2A_1 + E_1 + E_2$

Table 4. Enumeration of physical constants for crystals of axial symmetry

Group No.	6	18	12	25	7	19	14	26	1	4	16	9	22	2	5	17	11	23	8	20	15	27	3	21	24	
	C_{2v}	C_{3v}	C_{4v}	C_{6v}	D_2	D_3	D_4	D_6	C_1	C_2	C_3	C_4	C_6	C_1^i	C_2^i	C_3^i	C_4^i	C_6^i	D_2^i	D_3^i	D_4^i	D_6^i	C_1^h	C_3^h	D_3^h	
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
2	1	1	1	1	0	0	0	0	3	1	1	1	1	0	0	0	0	0	0	0	0	0	0	2	0	0
3, 3 (a)	3	2	2	2	3	2	2	2	6	4	2	2	2	6	4	2	2	2	3	2	2	2	2	2	0	0
4, 5	3	2	2	2	3	2	2	2	9	5	3	3	3	9	5	3	3	3	3	2	2	2	2	5	3	2
6	5	4	3	3	3	2	1	1	18	8	6	4	4	0	0	0	0	0	0	0	0	0	0	10	2	1
7	7	5	4	4	6	4	3	3	27	13	9	7	7	0	0	0	0	0	0	0	0	0	14	2	1	
8 (a)	9	6	6	5	9	6	6	5	21	13	7	7	5	21	13	7	7	5	9	6	6	5	13	5	5	
8	12	8	7	6	12	8	7	6	36	20	12	10	8	36	20	12	10	8	12	8	7	6	20	8	6	
9	15	10	8	7	15	10	8	7	54	28	18	14	12	54	28	18	14	12	15	10	8	7	28	12	7	
10	21	14	11	10	21	14	11	10	81	41	27	21	19	81	41	27	21	19	21	14	11	10	41	19	10	
11	17	13	10	8	12	8	5	3	63	29	21	15	11	0	0	0	0	0	0	0	0	0	34	10	5	
12	20	14	12	10	20	14	12	10	56	32	20	16	12	56	32	20	16	12	20	14	12	10	32	12	10	
13	39	26	22	17	39	26	22	17	126	68	42	34	24	126	68	42	34	24	39	26	22	17	68	24	17	
E	0	0	0	0	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	
O	1	0	0	0	3	2	2	2	6	4	2	2	2	0	0	0	0	0	0	0	0	0	2	0	0	

Table 5. Enumeration of physical constants for crystals of symmetry S_{4v} and S_4

No.	Representation	S_{4v}	13 S_{4v}	10 S_4
1	I	A_1	1	1
2	V	$B_1 + E_1$	0	0
3, 3 (a)	$[V^2]$	$2A_1 + B_1 + B_2 + E_1$	2	2
4, 5	V^2	$2A_1 + A_2 + B_1 + B_2 + 2E_1$	2	3
6	$V[V^2]$	$2A_1 + 2A_2 + 3B_1 + B_2 + 5E_1$	2	4
7	V^3	$3A_1 + 3A_2 + 4B_1 + 3B_2 + 7E_1$	3	6
8 (a)	$[[V^2]^2]$	$6A_1 + A_2 + 3B_1 + 3B_2 + 4E_1$	6	7
8	$[V^2]^2$	$7A_1 + 3A_2 + 5B_1 + 5B_2 + 8E_1$	7	10
9	$V^2[V^2]$	$8A_1 + 6A_2 + 7B_1 + 7B_2 + 13E_1$	8	14
10	V^4	$11A_1 + 10A_2 + 10B_1 + 10B_2 + 20E_1$	11	21
11	$V[[V^2]^2]$	$7A_1 + 7A_2 + 10B_1 + 5B_2 + 17E_1$	7	14
12	$[[V^2]^3]$	$12A_1 + 4A_2 + 8B_1 + 8B_2 + 12E_1$	12	16
13	$[V^2][[V^2]^2]$	$22A_1 + 12A_2 + 17B_1 + 17B_2 + 29E_1$	22	34
E	ϵ	B_2	0	0
O	$\epsilon[V^2]$	$A_1 + A_2 + 2B_2 + E_1$	1	2

(3) For C_p^i and D_p^i properties 2, 6, 7, 11, E and O change sign on inversion and hence give zero, others as for the groups C_p and D_p .

(4) For $C_1^h: E'_p = 2A'_1$,
 $C_3^h: E'_3, E'_6 \rightarrow 2A'_1$,
 $D_3^h: E'_3, E'_6 \rightarrow A'_1$.

Of the 32 crystallographic groups there remain only S_{4v} and S_4 . These could be treated by the Bhagavantam-Suryanarayana method quite easily but for completeness we give the reduced form of the representations for S_{4v} also in Table 5. Those for S_4 follow by identifying A_1 with A_2 (and B_1 with B_2).

We have in this way covered all the 32 crystal groups, and it may be verified that our results confirm in every

case those of Bhagavantam & Suryanarayana, their numbering of the groups being given in the above Tables above the Schoenflies symbol (which we have slightly modified in some cases). In addition we have derived the number of constants for a completely isotropic solid or for one having complete axial symmetry.

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