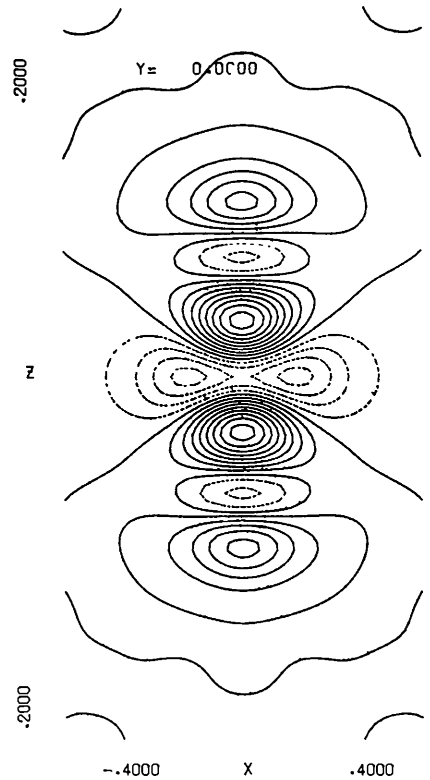

Fig. 3. Dynamic deformation density calculated with rigid-body thermal parameters as found in NaN_3. Contours at 0·05 e Å^{-3}.

Conclusions

We have shown that the time-averaged molecular electron density distribution for rigid-body librations can be obtained by a convolution of the molecular scattering factors with the distribution of orientations of the scattering vector **h**. The correct libration amplitude to be applied to two-center orbital products is found to be the motion of the center of density point, $\mathbf{r}_c$. Starting with a static molecular density, the dynamic density smeared by rigid-body translations and librations can be obtained for any magnitude of **T** and **L**.

The dynamic density obtained in this manner contains series termination effects, but for extended data sets the effects will be relatively small when the difference density, $\Delta\varrho_{\rm dyn}$, is calculated. In addition, if the object of calculating the dynamic density is for comparison with X-ray diffraction results, which are also obtained from a finite series, then series-termination effects may be included in the theory to the same extent as in the experiment. Although the results given here are for a linear molecule, the method is applicable to molecules of general geometry.

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Magnetic Properties of Crystals: An Alternative Method

By T. S. G. Krishnamurty, V. Appalanarasimham and K. Rama Mohana Rao
Andhra University, Waltair, S. India

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A method, based on the group-theoretical concept of the factor groups contained in a composition series, of obtaining the number of the constants required to describe a magnetic property in respect of the 90 magnetic point groups is described. The advantage of the method presented here is that one can enumerate simultaneously the constants needed for the description of the magnetic property for all the point groups involved in a composition series and their magnetic variants. Piezomagnetism is worked out in detail for one composition series.

1. Introduction

The character method developed by Bhagavantam (1942) has been successfully applied by Bhagavantam & Suryanarayana (1949), Bhagavantam & Pantulu (1964) and Bhagavantam (1966) for enumerating physical constants needed for the description of various physical properties in respect of the 90 magnetic symmetry groups. Jahn (1949), Juretschke (1951) and Fumi (1952*a*, *b*) have also made notable contributions to the methods of enumerating physical constants. In these methods, each one of the 90 magnetic symmetry groups has been separately dealt with for any physical property.

The 58 double-coloured point groups were rederived by Krishnamurty & Appalanarasimham (1974) who used the concept of composition series in their construction. Using a computed character to represent a magnetic property, we have explored the idea of the factor groups contained in a composition series to enumerate simultaneously the constants required to describe the magnetic property for all the point groups involved in the composition series and such of the magnetic variants which exist. The case of piezomagnetism is illustrated in this note for one composition series.

2. An alternative method

It is known that composition series (Lomont, 1959) exist among the 32 crystallographic point groups, which may be regarded as subgroups of one or the other of the point groups $m3m$ and $6/mmm$. A composition series for $m3m$ may be taken as

$$m3m \supset 432 \supset 23 \supset 222 \supset 2 \supset 1 \qquad (1)$$

with the composition factors 2, 2, 3, 2 and 2. Similarly a composition series for $6/mmm$ can be taken as

$$6/mmm \supset 622 \supset 6 \supset 3 \supset 1 \qquad (2)$$

with 2, 2, 2 and 3 as composition factors. It has been already shown (Krishnamurty & Gopala Krishnamurty, 1969) that the alternating representation of the factor group G/H, where H is a subgroup of index 2 of the point group G, engenders an alternating representation of G, which, in turn, induces a magnetic variant of G.

Piezomagnetism is the appearance of a magnetic moment $\mathbf{M}(M_i, i=1,2,3)$ on the application of a stress σ. The character (Bhagavantam & Pantulu, 1964) for piezomagnetism is given by

$$\chi_j'(R) = (4\cos^2\varphi \pm 2\cos\varphi)(1 \pm 2\cos\varphi), \qquad (3)$$

where the + or the − sign is to be taken according as the symmetry operation R is a pure rotation or a rotation-reflexion.

For any magnetic property, the character of a coset A_iH, where A_i belongs to G–H, in the factor group G/H may be defined as the sum of the characters of those elements of the group G, which are contained in the coset A_iH in respect of that magnetic property divided by the order of the coset.

Adopting this definition, we apply the following known formula (Bhagavantam & Venkatarayudu, 1969), to determine the number of piezomagnetic constants n_i appearing against the ith irreducible representation of a group G:

$$n_i = \frac{1}{N}\sum_j h_j \chi_j'(R)\chi_i(R). \qquad (4)$$

In equation (4), N is the total number of elements of the group G and h_j is the number of elements of the jth conjugacy class of G. $\chi_j'(R)$ is the computed character for piezomagnetism and is given by equation (3). $\chi_i(R)$ is the character of the symmetry operation R in the ith irreducible representation of G. The alternative method of enumeration of piezomagnetic constants presented here is illustrated below in six stages for the composition series (1).

(i) The point group 1 requires 18 piezomagnetic constants.

(ii) The character table of the factor group 2/1, which coincides with that of the point group 2, is

2/1	E	C_2	n_i
A	1	1	8
B	1	−1	10
$\chi'(R)$	18	−2	

So the point group 2 and its magnetic variant 2′, which are induced respectively by the irreducible representations A and B of the factor group 2/1, require eight and ten piezomagnetic constants.

(iii) Since the point group 2 is a normal subgroup of the point group 222, the group 222 can be written as the sum of the cosets 2 and $C_2'2$, *i.e.*, $222 = 2 + C_2'2$. Hence the factor group 222/2 has cosets 2 and $C_2'2$ as its elements and the character table of 222/2 is

222/2	2	$C_2'2$	n_i
A'	1	1	3
B'	1	−1	5
$\chi'(R)$	8	−2	

Since the point group 2 is the identity element in the factor group 222/2 and since eight piezomagnetic constants are needed for the point group 2, we take 8 as the character of the identity element in the factor group 222/2. The coset $C_2'2$ contains the elements C_2' and C_2'' and the character of each one of these elements in respect of piezomagnetism is −2 such that the character of the coset $C_2'2$ is −2 following the definition of the character of a coset introduced earlier. A similar procedure has been adopted with regard to the enumeration of the character of piezomagnetism for the elements of the factor groups 23/222, 432/23 and $m3m/432$, which are further needed for the considered composition series (1). From the point of view of cosets, the point groups 23, 432 and $m3m$ can be expressed as

$$23 = 222 + C_3 222 + C_3^2 222\,, \quad (5)$$

$$432 = 23 + C_2 23\,, \quad (6)$$

$$m3m = 432 + i432\,. \quad (7)$$

(iv) Since the characters of the cosets C_3222 and C_3^2222 are each equal to zero and that of 222 is 3 for piezomagnetism, we find that one piezomagnetic constant is required for the point group 23.

(v) The character tables of the factor groups 432/23 and $m3m/432$ are given below:

432/23	23	$C_2 23$	n_i
A''	1	1	0
B''	1	−1	1
$\chi'(R)$	1	−1	

The coset $C_2 23$ consists of the conjugacy classes 6 C_2 and 6 C_4. Their characters for piezomagnetism are respectively −12 and 0. Hence the character of the coset $C_2 23$ is −1. Thus, we find that the point group 432 and its magnetic variant $4'32'$ require respectively zero and one piezomagnetic constants.

(vi)

$m3m/432$	432	$i432$	n_i
A'''	1	1	0
B'''	1	−1	0
$\chi'(R)$	0	0	

Since piezomagnetism is a centrosymmetric property and the character of the identity element 432 in the factor group $m3m/432$ is zero, we infer readily that the character of the coset $i432$ in the factor group $m3m/432$ is also equal to zero. From the above character table, we observe that the crystal class $m3m$ and its variant $m'3m'$ do not require any constants for the description of piezomagnetism.

Thus, the point groups 1, 2, 222, 23, 432 and $m3m$ require respectively 18, 8, 3, 1, 0 and 0 piezomagnetic constants, whereas the associated magnetic point groups $2'$, $2'2'2$, $4'32'$ and $m'3m'$ need 10, 5, 1 and 0 constants to describe their piezomagnetic behaviour.

The results obtained here, by this method, in respect of piezomagnetism, for the point groups 1, 2, 222, 23, 432 and $m3m$ involved in the composition series (1) and their magnetic variants $2'$, $2'2'2$, $4'32'$ and $m'3'm'$ agree completely with those obtained by Bhagavantam & Pantulu (1964). This method can also be extended to any other magnetic or physical property.

3. Summary

The following points summarize the main results obtained in this paper.

(i) By the method outlined here, the physical constants needed to describe a physical property for all the point groups contained in a composition series and their magnetic variants can be obtained simultaneously; they need not be calculated separately for each of the point groups.

(ii) The idea of factor groups occurring in different composition series among the 32 crystallographic point groups can be utilized for the enumeration of physical constants in respect of all the 90 magnetic crystal classes.

(iii) It may be observed that, in general, the character of the coset A_iH, as defined here, for any physical property, in the factor group G/H, may not be equal to that of the element A_i.

(iv) For any physical property, it may be noted that the character of the coset A_iH in the factor group G/H should not numerically exceed that of H.

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