accordance with their estimated standard deviations, and theoretical structure factors were calculated using the scattering factors given in *International Tables for X-ray Crystallography* (1962). Initially a harmonic model was assumed and attempts to refine an extinction parameter resulted in a value not significantly different from zero, thus supporting the validity of the extinction correction procedure used. Values obtained for the temperature factors also agreed well with those given by Panke & Wölfel.

Anharmonic thermal vibration will affect primarily the high-angle odd-index reflexions with $h+k+l=4n\pm1$. Refinements using an anharmonic model, with B_{Mg} allowed to vary, resulted in values of β_{Mg} of about $-2{\cdot}5\times10^{-12}$ erg Å^{-3}, irrespective of the number of reflexions included in the analysis in addition to these more sensistive ones, and the other parameters were not changed significantly by the inclusion of the β parameter. It was found, however, that the reliability of the β_{Mg} value was improved by restricting the number of additional reflexions included, particularly since low angle reflexions are more dependent on such factors as the ionic charge and the outer electron distribution. A final analysis was therefore carried out using only the 13 highest-angle odd-index reflexions, *i.e.* from 751 onwards. A harmonic refinement varying only the scale factor, with the temperature factors fixed at the Panke & Wölfel values, gave good agreement with an R index of 0·96%, where

$$R=\Sigma||F_o|-|F_c||/|F_o|.$$

An anharmonic refinement, with only β_{Mg} varied and the scale factor fixed at the value obtained from the harmonic refinement resulted in a final value of $\beta_{Mg}=-2{\cdot}39(\pm0{\cdot}22)\times10^{-12}$ erg Å^{-3} and an R index of 0·79%. The experimental structure factors for these reflexions, together with the final calculated structure factors for the harmonic and anharmonic models are listed in Table 1.

It can be seen that, although the observed differences from the predictions of a harmonic model have little significance individually, they do, in all except two cases, have the sign predicted by the anharmonic model. In addition the agreement between observed and calculated structure factors is improved for all but two of the remaining reflexions. The significance of the overall improvement in the agreement resulting from the introduction of the anharmonicity parameter can be tested using statistical tables, for example those given by Hamilton (1965). The R index ratio in this case is 1·215, so that on the basis of these data the hypothesis that $\beta_{Mg}=0$ can be rejected at the 5% level, but not at the 2½% level.

Table 1. *Observed and calculated structure factors for* Mg_2Si

F_H and F_A are the calculated structure factors for the harmonic and anharmonic models respectively.

h	k	l	F_o	F_H	F_A
7	5	1	14·30	14·23	14·26
5	5	5	14·10	14·23	14·11
9	1	1	13·00	13·04	13·03
7	5	3	13·10	13·04	12·95
9	3	1	12·00	11·98	12·00
9	3	3	10·70	11·04	10·98
7	7	1	10·80	11·04	11·01
7	5	5	11·20	11·04	11·16
9	5	1	10·30	10·20	10·17
7	7	3	10·40	10·20	10·30
9	5	3	9·47	9·45	9·53
11	1	1	8·83	8·78	8·78
7	7	5	8·74	8·78	8·64

It is concluded, therefore, that the experimental data of Panke & Wölfel indicate the existence of an anharmonic contribution to the thermal vibration of the magnesium atoms, consistent with the tetrahedral site symmetry and of similar magnitude to that observed in other systems having the fluorite structure.

References

COOPER, M. J. (1970*a*). *Acta Cryst.* A**26**, 208.

COOPER, M. J. (1970*b*). *Thermal Neutron Diffraction*. Ed. B. T. M. WILLIS. Oxford Univ. Press.

COOPER, M. J. & ROUSE, K. D. (1968). *Acta Cryst.* A**24**, 405.

COOPER, M. J. & ROUSE, K. D. (1970). To be published.

COOPER, M. J., ROUSE, K. D. & WILLIS, B. T. M. (1968). *Acta Cryst.* A**24**, 484.

DAWSON, B., HURLEY, A. C. & MASLEN, V. W. (1967). *Proc. Roy. Soc.* A**298**, 289.

HAMILTON, W. C. (1965). *Acta Cryst.* **18**, 502.

International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.

PANKE, D. & WÖLFEL, E. (1968). *J. Appl. Cryst.* **1**, 255.

PANKE, D. & WÖLFEL, E. (1969). *Z. Kristallogr.* **129**, 9.

ROUSE, K. D., WILLIS, B. T. M. & PRYOR, A. W. (1968). *Acta Cryst.* B**24**, 117.

Acta Cryst. (1970). A**26**, 293

Magnetic symmetry and physical properties.

By T. S. G. KRISHNA MURTY and V. APPALANARASIMHAM, *Andhra University, Waltair, S. India*

(*Received* 11 *June* 1969 *and in revised form* 6 *October* 1969)

The number of independent non-vanishing constants required to describe the six known physical properties, involving a polar vector, has been determined by the character method of Bhagavantam & Suryanarayana for each one of the 58 double-coloured point groups.

Group theory has been successfully applied by Bhagavantam & Suryanarayana (1949), Jahn (1949) and recently by Koptsik (1966) to enumerate the constants needed to describe various physical or magnetic properties in crystals. More recently, a physical significance was given by Krishnamurty & Gopalakrishnamurty (1969*a*) to the number of constants, relating to a magnetic (or physical) property, appearing against the alternating representations of the 32 point groups. Following this, the number of second-, third- and the fourth-order elastic coefficients for each of the 58 double-coloured point groups have been enlisted by Krishnamurty & Gopalakrishnamurty (1969*b*).

In this note, the number of constants needed to describe some of the known physical properties is enumerated for the 58 magnetic variants of the 32 point groups on the basis of physical significance (1969*a*). The results given here are new and were not considered by Turov (1965).

Only those physical properties with serial numbers 2,3,5,8,11 and 13 in Table 7*a* of Bhagavantam (1966) are considered here, and those properties which have no known physical significance are omitted. It is known (Bhagavantam, 1966) that ferromagnetism is possible only in those crystal classes in which pyromagnetism is also possible; there are 31 ferromagnetic classes. These 31 classes consist of 12 conventional point groups and 19 double-coloured point groups. That is to say, a magnetic property such as pyromagnetism is exhibited by 12 conventional crystal classes. Whether or not the converse is true and whether the 58 double-coloured crystal classes exihibit non-magnetic properties are investigated in this note for the six physical properties. The numbers obtained in respect of these properties by means of the character method of Bhagavantam & Suryanarayana (1949) are given in Table 1 for the 58 double-coloured crystal classes.

Table 1. *The physical property numbers of the* 58 *double-coloured crystal classes*

Number	Double-coloured point groups in international symbols	Physical properties 2	3	5	8	11	13
1	$\bar{1}'$	3	–	18	–	63	–
2	m'	1	2	8	16	29	58
3	$2'$	2	2	10	16	34	58
4	$2'/m$	2	–	10	–	34	–
5	$2/m'$	1	–	8	–	29	–
6	$2'/m'$	–	2	–	16	–	58
7	$2'mm'$	1	1	5	8	17	29
8	$2m'm'$	–	1	3	8	12	29
9	$2'2'2$	1	1	5	8	17	29
10	$m'mm$	1	–	5	–	17	–
11	$m'm'm'$	–	–	3	–	12	–
12	$mm'm'$	–	1	–	8	–	29
13	$4'$	–	2	4	10	14	34
14	$\bar{4}'$	1	2	4	10	15	34
15	$4'/m'$	–	–	4	–	14	–
16	$4/m'$	1	–	4	–	15	–
17	$4'/m$	–	2	–	10	–	34
18	$4m'm'$	–	–	1	3	5	12
19	$4'mm'$	–	1	2	5	7	17
20	$\bar{4}'2m'$	–	1	1	5	5	17
21	$\bar{4}'2'm$	1	1	3	5	10	17
22	$\bar{4}2'm'$	–	–	2	3	7	12
23	$42'2'$	1	–	3	3	10	12
24	$\bar{4}22'$	–	1	2	5	7	17
25	$4'/m'mm'$	–	–	2	–	7	–
26	$4/m'mm$	1	–	3	–	10	–
27	$4/mm'm'$	–	–	–	3	–	12
28	$4/m'm'm'$	–	–	1	–	5	–
29	$4'/mmm'$	–	1	–	5	–	17
30	$\bar{3}'$	1	–	6	–	21	–
31	$3m'$	–	–	2	4	8	16
32	$32'$	1	–	4	4	13	16
33	$\bar{3}m'$	–	–	–	4	–	16
34	$\bar{3}'m$	1	–	4	–	13	–
35	$\bar{3}'m'$	–	–	2	–	8	–
36	$\bar{6}'$	1	–	4	4	11	18
37	$6'$	–	–	2	4	10	18
38	$6/m'$	1	–	4	–	11	–
39	$6'/m$	–	–	2	–	10	–
40	$6'/m'$	–	–	–	4	–	18
41	$\bar{6}m'2'$	–	–	1	2	5	7
42	$\bar{6}'m2'$	1	–	3	2	8	9
43	$\bar{6}'m'2$	–	–	1	2	3	9
44	$6m'm'$	–	–	1	2	3	7
45	$6'm'm$	–	–	1	2	5	9
46	$62'2'$	1	–	3	2	8	7
47	$6'22'$	–	–	1	2	5	9
48	$6/m'mm$	1	–	3	–	8	–
49	$6/mm'm'$	–	–	–	2	–	7
50	$6/m'm'm'$	–	–	1	–	3	–
51	$6'/mmm'$	–	–	1	–	5	–
52	$6'/m'mm'$	–	–	–	2	–	9
53	$m'3$	–	–	1	–	4	–
54	$\bar{4}'3m'$	–	–	–	1	1	4
55	$4'32'$	–	–	1	1	3	4
56	$m'3m'$	–	–	–	–	1	–
57	$m3m'$	–	–	–	1	–	4
58	$m'3m$	–	–	1	–	3	–

Bhagavantam (1966) implies that a symmetry operation and its complement will have the same effect on physical properties such as elasticity, photoelasticity, *etc*. This book gives the impression that there is no distinction between a point group and its magnetic variants so far as the physical properties are concerned: for instance, according to Bhagavantam, in the case of photoelasticity the crystal class $2mm$ and its variants $2m'm'$ and $2'mm'$ require the same 12 constants, where as, in the light of this paper, the above three classes require 12,8 and 8 constants respectively (Table 1), which are different in nature.

These physical properties are in general exihibited by crystals in the magnetic state. However, in the magnetic state the number of constants required differs from that required in the ordinary state. This work suggests that experimental determination of the physical constants of crystals in the magnetic state is advisable.

The authors wish to express their sincere thanks to Professor T. Venkatarayudu for his kind interest in this work.

References

BHAGAVANTAM, S. & SURYANARAYANA, D. (1949). *Acta Cryst.* **2**, 21.

BHAGAVANTAM, S. (1966). *Crystal Symmetry and Physical Properties*. London: Academic Press.

JAHN, H. A. (1949). *Acta Cryst.* **2**, 30.

KOPTSIK, V. A. (1966). *Shubnikovskie Gruppy*, p.65. Moscow Univ. Press.

KRISHNAMURTY, T. S. G. & GOPALAKRISHNAMURTY, P. (1969*a*). *Acta Cryst.* A**25**, 329.

KRISHNAMURTY, T. S. G. & GOPALAKRISHNAMURTY, P. (1969*b*). *Cur. Sci. India*, **38**, 102.

TUROV, E. A. (1965). *Physical Properties of Magnetically Ordered Crystals*. London: Academic Press.