In Fig. 1 the broken line represents the variation with temperature of $V^{\frac{1}{3}}$, where V ($= 0{\cdot}866\ ca^2$) is the structure cell volume. The slope of this curve is approximately uniform and the curve passes smoothly through the transition region in the neighbourhood of 400° C.

Discussion

In CrSb the magnetic atoms (Cr) are arranged in plane sheets perpendicular to [0001]. The results just described indicate that the distance between these sheets decreases anomalously as the temperature is lowered through the transition point. This effect takes place without any sudden change of structure cell volume or change of crystal symmetry. According to Snow (1952) the magnetic moments of the chromium atoms in a given (0001) plane are all parallel, but moments in neighbouring planes are antiparallel. Thus the antiferromagnetic exchange forces are directed predominantly along the [0001] direction, an interpretation which is strongly supported by the present work.

It is interesting to note that MnTe, which is also an antiferromagnetic compound with the NiAs-type structure, undergoes a similar decrease of c/a (Greenwald, 1952) on being cooled through the transition temperature near 35° C. The magnitude of the change for MnTe is, however, considerably smaller than in CrSb.

The transition temperature of CrSb has been variously reported as 400° C. (Foëx & Graaf, 1939) and 450° C. (Snow, 1952). It is not possible to obtain a more precise value from the shape of the magnetic susceptibility–temperature curve, as the maximum in this curve is exceptionally broad. If we assume that the lattice changes in CrSb appear as soon as the temperature falls below T_λ, we can determine the value of T_λ from Fig. 1 as 420±10° C.

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Enumeration of physical constants of crystals.

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Bhagavantam & Suryanarayana (1949) have given a method by which the number of constants necessary to specify different physical properties of crystals can be directly obtained by using a group theoretical formula which gives the number of times a certain irreducible representation of a group appears in a given representation; these authors have considered all the 32 crystal classes. An alternative method for the same purpose has been given by Jahn (1949) whose results confirm in every case those of Bhagavantam & Suryanarayana; in addition Jahn has also considered the case of a body with complete axial symmetry, his group R_∞, and one with complete axial symmetry together with an inversion, his group R^i_∞. The result for these two cases are given by Jahn in his Table 1 (where the heading for the fifth column has been misprinted: it should be R_∞ instead of R^i_∞). Jahn has further considered the groups C_∞, $C_{\infty v}$, D_∞ etc.

For the sake of completeness, an effort has been made to extend the method of Bhagavantam & Suryanarayana to give the number of constants where the symmetry group is no longer finite, making it necessary to use group integration instead of a finite summation in the formula mentioned above.

In the following we shall consider the groups which in the notation of Jahn are R_∞, R^i_∞, C_∞, $C_{\infty v}$, C^h_∞, D_∞ and D^h_∞. For the first two we need integration over the group of all orthogonal transformations in three dimensions for which the 'volume element' is $\sin^2\frac{1}{2}\varphi d\varphi$, $0 \leqslant \varphi \leqslant \pi$, while for the rest the integration is essentially over a group of orthogonal transformations in two dimensions for which the 'volume element' is simply $d\varphi$, $0 \leqslant \varphi \leqslant 2\pi$. Let $\chi(\varphi)$ denote the character of a rotation φ about an axis and $\psi(\varphi)$ that of a rotation–reflexion φ. These are given in Table 1 of Bhagavantam & Suryanarayana; we need not specify the direction of the axis of rotation because the characters of the representations we are concerned with depend only on φ.

The required numbers are then obtained from the following formulae:

$$(1)\qquad R_\infty,\ n = \int_0^\pi \chi(\varphi)\sin^2\tfrac{1}{2}\varphi d\varphi \Big/ \int_0^\pi \sin^2\tfrac{1}{2}\varphi d\varphi\ ,$$

$$(2)\qquad R^i_\infty,\ n = \int_0^\pi [\chi(\varphi)\pm\psi(\pi-\varphi)]\sin^2\tfrac{1}{2}\varphi d\varphi \Big/ 2\int_0^\pi \sin^2\tfrac{1}{2}\varphi d\varphi\ ,$$

$$(3)\qquad C_\infty,\ n = \int_0^{2\pi} \chi(\varphi)d\varphi \Big/ \int_0^{2\pi} d\varphi\ ,$$

$$(4)\qquad C_{\infty v},\ n = \int_0^{2\pi} [\chi(\varphi)\pm\psi(0)]d\varphi \Big/ 2\int_0^{2\pi} d\varphi\ ,$$

$$(5)\qquad C^h_\infty,\ n = \int_0^{2\pi} [\chi(\varphi)\pm\psi(\varphi)]d\varphi \Big/ 2\int_0^{2\pi} d\varphi\ ,$$

$$(6)\qquad D_\infty,\ n = \int_0^{2\pi} [\chi(\varphi)+\chi(\pi)]d\varphi \Big/ 2\int_0^{2\pi} d\varphi\ ,$$

$$(7)\qquad D^h_\infty,\ n = \int_0^{2\pi} [\chi(\varphi)\pm\psi(\varphi)+\chi(\pi)\pm\psi(0)] \Big/ 4\int_0^{2\pi} d\varphi\ ,$$

Table 1

No.	Symmetry	1	2	3, 3*a*	4, 5	6	7	8*a*	8	9	10	11	12	13	En.	O.A.
33	R_∞	1	0	1	1	0	1	2	2	2	3	0	3	4	1	1
34	R^i_∞	1	0	1	1·	0	0	2	2	2	3	0	3	4	0	0
35	C_∞	1	1	2	3	4	7	5	8	12	19	11	10	22	1	2
36	$C_{\infty v}$	1	1	2	2	3	4	5	6	7	10	8	9	16	0	0
37	C^h_∞	1	0	2	3	0	0	5	8	12	19	0	10	22	0	0
38	D_∞	1	0	2	2	1	3	5	6	7	10	3	9	16	1	2
39	D^h_∞	1	0	2	2	0	0	5	6	7	10	0	9	16	0	0

where the negative sign has to be taken with ψ in the case of optical activity and enantiomorphism.

Using $\chi(\varphi)$ and $\psi(\varphi)$ from Table 1 of Bhagavantam & Suryanarayana in the above formulae we get the integers shown in Table 1, which can be placed at the bottom of their Table 2.

These results are all in agreement with those of Jahn in the paper already mentioned.

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Three-dimensional Fourier summations on a high-speed digital computer.

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The application of digital computers to crystal-structure investigation has been receiving increased attention concomitant with the further development and increased availability of such computers (Bennett & Kendrew, 1952; Ordway, 1950, 1952; Shoemaker, 1952). We have been using the National Bureau of Standards Western Automatic Computer (Huskey, 1950) in calculations for our studies of the structures of sulfamide (Mayer & Trueblood, 1953) and cyclopropylamine hydrochloride. Three-dimensional Fourier summations over one-sixteenth of the unit cell of sulfamide, including all of the 180 observed reflections from this crystal (space group *Fdd*2), have been carried out in less than 35 min. of computing time. Because the asymmetric unit for sulfamide is contained in one-sixteenth of the unit cell the time required for computing was less than can ordinarily be expected, but it is estimated that in most cases not more than 90 min. would be needed.

Data is fed into the computer on I.B.M. cards at the rate of 240 cards per minute. Each card holds the required data for ten spectra—the indices, observed structure factors and calculated phases. (The structure factors were also calculated on the computer.) These cards, containing information in the binary system, are prepared automatically from decimally punched cards. Several duplicate packs of the cards are prepared to expedite the necessary recycling operations. The Fourier summation is then carried out in the machine as a programmed sequence of basic operations. The memory of the computer at present holds 256 36-digit binary numbers; the machine performs such operations as addition and subtraction at the rate of more than nine hundred thousand per minute. Computed results are punched decimally on I.B.M. cards, at a maximum rate of fifty cards per minute. Each card contains fifteen values of the electron density; in sulfamide, this corresponds to one line (fifteen one-sixtieths) in the (x, y) grid at a constant value of z. Upon completion of the map for one z plane, an increment is automatically added to z, and the cycle of programmed calculations is repeated until the electron-density distribution has been calculated over the desired range of z.

Although the interval now employed for the grid of the electron-density map is 1/60 of the unit cell edge, it is feasible to change the interval to 1/120 or 1/30. The Fourier equations employed are of the type in which all the indices are positive (Lonsdale, 1936). Although we have to date programmed only for space groups *Fdd*2 and $Pbn2_1$, our programming may easily be extended to any space group for which the summation terms can conveniently be put into the form

$$\pm \sum_0^k \sum_0^h \sum_0^l |F_{hkl}| \, \genfrac{}{}{0pt}{}{\cos}{\sin} 2\pi(lz-\alpha) \cdot \genfrac{}{}{0pt}{}{\cos}{\sin} 2\pi hx \cdot \genfrac{}{}{0pt}{}{\cos}{\sin} 2\pi ky \, .$$

Three-dimensional Patterson functions can of course be rapidly computed in a similar fashion. We expect to present a fuller description of these computing procedures with an account of the structure of sulfamide when our investigation of this substance has been completed.

We wish to express our gratitude to the Institute for Numerical Analysis of the National Bureau of Standards on this campus for the use of the SWAC and other computing facilities.

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