The Crystal Structure of Nickel Sulphate Hexahydrate, $NiSO_4 \cdot 6H_2O$.

By

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(With 5 figures.)

1. Introduction.

The analysis of this crystal was initially undertaken in the hope of proving a clue to the structure of the heptahydrate of nickel-sulphate $(NiSO_4 \cdot 7H_2O)$, which is interesting as an example of a paramagnetic crystal. However, although the complete structure of the heptahydrate is not yet known, the structure of the hexahydrate is in itself of sufficient interest to warrant publication.

$NiSO_4 \cdot 6H_2O$ crystallises in two modifications, one belonging to the tetragonal system, and the other to the monoclinic system. This research deals only with the tetragonal form.

2. Crystallography.

Crystals of $NiSO_4 \cdot 6H_2O$ may be grown from an acid solution of nickel sulphate. The tetragonal modification is formed by slow evaporation at ordinary temperatures, while the monoclinic modification is formed at higher temperatures. The tetragonal crystal belongs to the trapezohedral class, and its axial ratios are given by Groth[1]) as

$$a : c = 1 : 1.912.$$

The most frequently occurring forms are {001} and {111}. The crystals are usually tabular parallel to (001) and cleavage is very good parallel to this plane.

3. Unit Cell, Lattice, and Space Group.

Rotation photographs taken with approximately cylindrical crystals showed that the c spacing was 18.3 Å, and the a spacing 9.61 Å. All

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1) Groth, Chem. Kryst. 2, 423.

spots having $h + k$ odd were found to be absent, indicating a centring of the squared faces of the unit cell. In order to minimize the labour of analysing the rotation photographs, therefore, the a and b axes were rotated through $45°$, so as to use the simpler unit cell. Rotation photographs about the new a and b axes verified that the new value of a_0 was equal to

$$9.61 \,/\, \sqrt{2} = 6.80 \text{ Å}.$$

The unit cell has therefore a volume of

$$6.8 \times 6.8 \times 18.3 \text{ Å}^3.$$

Now the mean of the specific-gravity determinations recorded by Groth is 2.07, so that the number of molecules of $NiSO_4 \cdot 6 H_2O$ in the unit cell turns out to be four.

The rotation photographs show many spots for which $h + k + l$ is odd, so that the lattice is the simple tetragonal lattice Γ_t.

The following tables give the intensities of the orders of (001) and (100), the intensities being placed in the eight classes: very-strong (v-s), strong (s), medium-strong (m-s), medium (m), weak-medium (w-m), weak (w), very-weak (v), and zero (0).

Table I.
Observed intensities of (h00).

h	1	2	3	4	5	6	7	8
Strength	0	s	0	w	0	0	0	w-m

Table II.
Observed intensities of (00l).

l	1	2	3	4	5	6	7	8	9	10	11
Strength	0	0	0	v. s	0	0	0	v	0	0	0

l	12	13	14	15	16	17	18	19	20	21	22
Strength	s	0	0	0	m-s	0	0	0	m-s	0	0

The (100) spacing is therefore halved and the (001) spacing quartered.

The space group is therefore D_4^4 or D_4^8, these space groups being enantiomorphous[1]). The symmetry elements of the structure are shown in figure 1, which is a copy of the Astbury and Yardley figure no. 116, with a shift of $\frac{1}{2} a_0$.

The equivalent points of D_4^4 are as follows:

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1) Astbury and Yardley, Phil. Trans. **224**, 221. 1924.

Four equivalent points:

a) $(u\,u\,0)$ $(\bar{u}\,\bar{u}\,\tfrac{1}{2})$ $(\tfrac{1}{2}+u,\tfrac{1}{2}-u,\tfrac{3}{4})$ $(\tfrac{1}{2}-u,\tfrac{1}{2}+u,\tfrac{1}{4})$

Eight equivalent points:

b) $(x\,y\,z)$ $(\tfrac{1}{2}+y,\tfrac{1}{2}-x,\tfrac{3}{4}+z)$ $(\bar{x}\,\bar{y}\,\tfrac{1}{2}+z)$ $(\tfrac{1}{2}-y,\tfrac{1}{2}+x,\tfrac{1}{4}+z)$
$(\tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{4}-z)$ $(\bar{y}\,\bar{x}\,\tfrac{1}{2}-z)$ $(\tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{3}{4}-z)$ $(y\,x\,\bar{z})$.
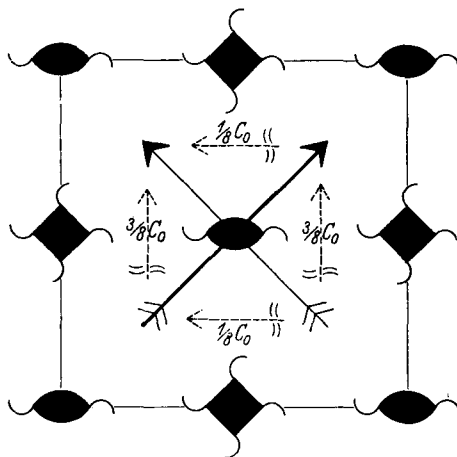

Fig. 1. The symmetry elements of D_4^4.

4. The Crystal Structure : Preliminary Considerations.

It follows that the Ni and S atoms must lie on the positions a), i. e. on the dyad rotation axes of the cell.

The sulphate oxygens must build up into tetrahedra around the sulphur, and the tetrahedra must have their rotation axes coincident with the rotation axes of the structure. Thus none of the sulphate oxygens lies on the rotation axes; they must be in two sets of eight given by the positions b) with two sets of parameters $(x\,y\,z)$.

There are twenty-four water molecules in the unit cell. If we take the distance between sulphate oxygens to be 2.5 Å, between sulphate oxygen and water to be 2.7 Å, and between water and nickel to be 2.1 Å, then if we put two water molecules on the rotation axes the length of the diagonal of the unit cell would need to be 10.7 Å instead of 9.61 Å. There cannot therefore be two sets of water molecules on a). Since there cannot be only one set of waters in special positions the twenty-four must lie on three sets of the general positions b).

Thus for the complete definition of the structure we require 17 parameters, one each for the Ni and S, six for the sulphate oxygens, and nine for the water molecules.

The structure factors for the arrangement then become, if the nickel parameter is taken as u and the sulphur parameter as v, and if the summation of the general term is taken over the five sets of (xyz) parameters:

Class 1. $l/2$ even, $h + k$ even:

$$\{4Ni \cdot \cos hu \cdot \cos ku + 4S \cdot \cos hv \cdot \cos kv$$
$$+ 4O \, \Sigma \, (\cos hx \cdot \cos ky + \cos hy \cdot \cos kx) \cos lz\}^2$$
$$+ \{4O \, \Sigma \, (\sin hx \cdot \sin ky - \sin hy \cdot \sin kx) \sin lz\}^2.$$

Class 2. $l/2$ even, $h + k$ odd:

$$\{4Ni \cdot \sin hu \cdot \sin ku + 4S \cdot \sin hv \cdot \sin kv$$
$$+ 4O \, \Sigma \, (\sin hx \cdot \sin ky + \sin hy \cdot \sin kx) \cos lz\}^2$$
$$+ \{4O \, \Sigma \, (\cos hx \cdot \cos ky - \cos hy \cdot \cos kx) \sin lz\}^2.$$

Class 3. $l/2$ odd, $h + k$ even:

$$\{4Ni \cdot \sin hu \cdot \sin ku + 4S \cdot \sin hv \cdot \sin kv$$
$$+ 4O \, \Sigma \, (\sin hx \cdot \sin ky + \sin hy \cdot \sin kx) \cos lz\}^2$$
$$+ \{4O \, \Sigma \, (\cos hx \cdot \cos ky - \cos hy \cdot \cos kx) \sin lz\}^2.$$

Class 4. $l/2$ odd, $h + k$ odd.

$$\{4Ni \cdot \cos hu \cdot \cos ku + 4S \cdot \cos hv \cdot \cos kv$$
$$+ 4O \, \Sigma \, (\cos hx \cdot \cos ky + \cos hy \cdot \cos kx) \cos lz\}^2$$
$$+ \{4O \, \Sigma \, (\sin hx \cdot \sin ky - \sin hy \cdot \sin kx) \sin lz\}^2.$$

Class 5. $l = 4n + 1$, $h + k$ even:

$$[2Ni \cdot \sin (h - k)u + 2S \cdot \sin (h - k)v$$
$$+ 2O \, \Sigma \, \{\sin (hx - ky) \cdot \cos lz - \sin (hx + ky) \cdot \sin lz$$
$$+ \sin (hy + kx) \cdot \sin lz + \sin (hy - kx) \cdot \cos lz\}]^2$$
$$+ [2Ni \cdot \sin (h + k)u + 2S \cdot \sin (h + k)v$$
$$+ 2O \, \Sigma \, \{\sin (hx + ky) \cdot \cos lz + \sin (hy - kx) \cdot \sin lz$$
$$- \sin (hx - ky) \cdot \sin lz + \sin (hy + kx) \cdot \cos lz\}]^2.$$

Class 6. $l = 4n + 1$, $h + k$ odd:

$$[- 2Ni \cdot \sin (h - k)u - 2S \cdot \sin (h - k)v$$
$$+ 2O \, \Sigma \, \{- \sin (hx + ky) \cdot \sin lz - \sin (hy - kx) \cdot \cos lz$$
$$+ \sin (- hx + ky) \cdot \cos lz + \sin (hy + kx) \cdot \sin lz\}]^2$$
$$+ [2Ni \cdot \sin (h + k)u + 2S \cdot \sin (h + k)v$$
$$+ 2O \, \Sigma \, \{\sin (hx + ky) \cdot \cos lz - \sin (hy - kx) \cdot \sin lz$$
$$+ \sin (hy + kx) \cdot \cos lz + \sin (hx - ky) \cdot \sin lz\}]^2.$$

Class 7. $l = 4n + 3$, $h + k$ even:

$$[- 2Ni \sin (h - k)u - 2S \cdot \sin (h - k)v$$
$$+ 2O\, \Sigma \{- \sin (hx + ky) \cdot \sin lz - \sin (hy - kx) \cdot \cos lz$$
$$- \sin (hx - ky) \cdot \cos lz + \sin (hy + kx) \cdot \sin lz\}]^2$$
$$+ [2Ni \cdot \sin (h + k)u + 2S \cdot \sin (h + k)v$$
$$+ 2O\, \Sigma \{\sin (hx + ky) \cdot \cos lz - \sin (hy - kx) \cdot \sin lz$$
$$+ \sin (hx - ky) \cdot \sin lz + \sin (hy + kx) \cdot \cos lz\}]^2.$$

Class 8. $l = 4n + 3$, $h + k$ odd:

$$[2Ni \cdot \sin (h - k)u + 2S \cdot \sin (h - k)v$$
$$+ 2O\, \Sigma \{- \sin \cdot (hx + ky) \cdot \sin lz + \sin (hy - kx) \cdot \cos lz$$
$$- \sin (- hx + ky) \cdot \cos lz + \sin (hy + kx) \cdot \sin lz\}]^2$$
$$+ [2Ni \cdot \sin (h + k)u + 2S \cdot \sin (h + k)v$$
$$+ 2O\, \Sigma \{\sin (hx + ky) \cdot \cos lz + \sin (hy - kx) \cdot \sin lz$$
$$+ \sin (hy + kx) \cdot \cos lz - \sin (hx - ky) \cdot \sin lz\}]^2.$$

5. Location of the Nickel and Sulphur Atoms.

Tables of the intensities of the observed spots show that reflections from planes for which $h + k$ is odd are usually very weak. For example the planes of table III ($h + k$ even) may be compared with those of

Table III. Intensities of planes of class 1.

| | | | | l | | | | Calculated Intensities. | | |
| | | | | | | | | Value of u | | |
h	k	0	4	8	12	16	20	.70	.71	.72
0	2	s	m-s	s, m-s	m	—	m	.66	.78	.88
0	4	w	w-m	w-m	0	w	—	.10	.29	.55
0	6	0	0	0	—	—	—	.09	.00	.18
0	8	w	w-m	—	—	—	—	.64	.17	.00
1	1	0	0	w-m	w	—	0	.00	.00	.00
1	3	w	w-m	v	v	v, 0	0	.06	.02	.01
1	5	v	w, v	v	0	0	—	.09	.05	.02
1	7	0	v	v	—	—	—	.06	.06	.03
2	2	0	m, m-s	m	m, w-m	—	—	.42	.61	.78
2	4	m	w, w-m	w, w-m	—	w	—	.06	.23	.49
2	6	v	0	v	—	—	—	.06	.00	.13
3	3	m	· w	w	w	—	—	.41	.21	.15
3	5	w-m	m	w-m, w	—	—	—	.64	.42	.19
3	7	w	w-m	0	—	—	—	.41	.46	.27
4	4	w-m	v	0	—	—	—	.01	.08	.30
4	6	0	0	—	—	—	—	.01	.00	.15
5	5	m-s	—	m	—	—	—	1.00	.81	.43

Table IV.

Intensities of planes of class 2.

h	k	0	4	8	12	16	20
					l		
1	2	w-m	m	m-s, m	—	0	—
1	4	0	—	v	—	—	—
1	6	v	0	v	—	—	—
1	8	m	0	—	—	—	—
2	3	m, w-m	v	0	v	0	—
2	5	v	0	0	—	—	—
2	7	0	0	0	—	—	—
3	4	w-m	v	0	v	—	—
3	6	0	v	v	—	—	—
3	8	0	—	—	—	—	—
4	5	0	0	—	—	—	—
4	7	v	—	—	—	—	—
5	6	0	0	—	—	—	—
0	1	—	0	w-m	w	w	v
0	3	—	m	0	v	0	0
0	5	—	v	0	0	—	—
0	7	—	0	0	0	—	—

table IV ($h + k$ odd). This means that the Ni and S parameters must differ by .5, so that the (001) square of the Ni lattice is centred by the S atoms. The f-values of Ni and S are approximately in the ratio $2:1$, so that the maximum possible intensities with $h + k$ odd is one ninth of those with $h + k$ even. Since the weakness of the $h + k$ odd planes holds for all values of sin θ we may assume that the parameters u and v differ by exactly .5. One parameter, u, will now determine both u and v.

The value of u may best be found from a study of planes for which $h + k$ is even. The structure-factors for these planes, neglecting the oxygen influence, involve only h and k, and thus planes in each class with the same value of h and k may be grouped together. Members of such a group of planes will have similar intensities with some exceptions due to the occasional adding-together of the oxygens (especially at small values of sin θ). These exceptional values may be disregarded and the Ni and S contribution is obtained alone. It now remains only to find a value of the parameter u which will give the correct Ni and S contributions.

The structure-factor for the planes of class 1 reduces to

$$[4 (Ni + S) \cos hu \cdot \cos ku]^2$$

and the observed intensities for the planes of this class are recorded in table III. The last three columns of this table give the values of $\cos^2 hu$ $\cdot \cos^2 ku$ for values of u .70, .71 and .72. It may easily be seen that the value

$$u = .71$$

gives the best correspondence between observation and calculation. The other classes of planes give the same result, so that we may take the parameters as .71 for the nickel, and .21 for the sulphur.

6. Location of the Oxygen Atoms and Water Molecules.

We shall assume that the SO_4 groups are tetrahedral, with an 0 — 0 distance of 2.5 Å, so that the parameters of the two sets of oxygen atoms must be related so as to give these tetrahedra, of which the orientation is as yet undefined.

The water molecules would be expected to group around the metal atoms, as was found to occur in the case of beryllium sulphate tetra-hydrate[1]) and it is probable that they will lie at the corners of a regular octahedron with the Ni at the centre. If the diameter of the water mole-cule is taken to be 2.8 Å, then the distance from Ni to H_2O on the octa-hedral structure is $2.8/\sqrt{2} = 2.0$ Å, which is satisfactory. The octahedron must lie with the rotation axis of the cell passing through the mid-points of opposite sides, and its orientation about this axis has now to be deter-mined from considerations of "fit", and from X-ray reflection intensities.

First of all the probable orientation of the water octahedron with respect to the sulphate groups on the same rotation axis may be found. The most favourable case is that illustrated in figure 2 which shows an
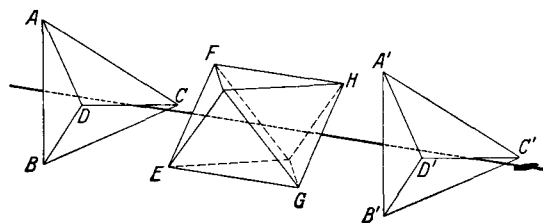

Fig. 2. Octahedra and tetrahedra on the same axis.

octahedron and two adjacent identical tetrahedra. The edge CD of the tetrahedron is rotated through 45° with respect to the edge EF of the octahedron, and on this arrangement the distances ED and $A'H$

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1) Beevers and Lipson, Z. Krist. 82, 297. 1932.

may be calculated to be each 2.7 Å. Now one of these distances can only be increased at the expense of the other and since it is unlikely that the distance from oxygen to water should be less than 2.7 Å the relative orientation of tetrahedron and octahedron is either that shown in figure 2, or that shown in figure 2 with a relative rotation of one of the solids through 90°.

A model was built, to a scale of about one inch to the Ångstrom unit, in order to consider the "fit" of the octahedra and tetrahedra on neighbouring rotation axes, but the fit seemed fairly good for a number of angular positions of the groups, owing to the uncertainty in the water diameter. The final adjustments were therefore made from the X-ray intensities of certain planes, namely those for which the Ni and S contribution is zero. These are the planes of classes 2 and 4 with $h = 0$. The structure-factors are then

$$\Sigma O \; (\cos ky - \cos kx) \sin lz.$$

The contribution of the water molecules (which were given the oxygen f-curves) was evaluated for different orientations of the octahedron. It was found that with an edge such as EF of the octahedron at 45° to the (001) plane (figure 2), the contribution from the waters alone was in excellent agreement with observed intensities. Now there are two positions of the tetrahedra which give zero contribution to these planes, one of which has an edge such as AB horizontal and the other has this edge vertical. With the 45° position of the octahedron one of these positions gives excellent intensities throughout, while the other gives some bad discrepancies. It was therefore concluded that the first of these positions gives the correct structure.

The arrangement has the parameters, for the waters

.67	.45	.054	. . . . 1.
.97	.75	.054	. . . . 2.
.56	.86	.077	. . . . 3.

and for the oxygens

.12	.12	.068	. . . . 4.
.43	.17	.000	. . . . 5.

The calculated intensities with these parameters are listed in table 5. The table includes planes, in order of θ, of the following types:

Class 1, with $h = 0$, with $h = k$, with $l = 0$.
Class 2, with $h = 0$, with $l = 0$.
Class 3, with $h = 0$, with $h = k$.

Class 4, with $h = 0$.
Class 5, with $h = k$.
Class 7, with $h = k$.

The structure-factors of these planes are much simpler than in the general cases, and table V provides a sufficient proof of the assigned structure.

The f-curves of James and Brindley[1] were used in the calculations.

Table V.
Comparison of intensities.

Plane			Observed	Calculated	Plane			Observed	Calculated
h	k	l			h	k	l		
0	1	2	v	1,800	0	1	10	w	430
1	1	0	0	80	2	2	7	w	2,100
0	0	4	v-s	200,000	1	1	10	s	21,000
1	1	1	m	9,200	0	4	0	w	820
1	1	2	s	180,000	2	2	8	m	20,000
1	0	4	0	20	0	4	2	0	6
1	1	3	m	7,400	1	4	0	0	400
1	1	4	0	64	0	3	8	0	150
0	2	0	s	36,000	0	4	4	w-m	4,400
0	2	2	m	3,500	3	3	0	m	5,400
1	2	0	w-m	2,700	3	3	1	m	6,000
1	1	5	m	4,500	3	3	2	w	5,400
0	2	4	s	44,000	1	1	11	v	540
0	1	6	m, w-m	5,100	2	2	9	w	1,400
1	1	6	m-s	33,000	3	3	3	w	1,700
2	2	0	0	690	3	3	4	w	3,000
2	2	1	w	1,900	2	4	0	m	5,300
2	2	2	0	42	0	0	12	s	23,000
0	2	6	0	500	3	3	5	w	3,100
2	2	3	0	200	0	4	6	0	100
1	1	7	w, w-m	2,100	0	3	10	v	20
0	0	8	v	630	3	3	6	w	1,000
0	1	8	w-m	2,700	2	2	11	w-m	4,700
0	3	2	0	160	0	2	12	m	7,500
2	2	4	m, m-s	12,000	0	4	8	w-m	3,300
1	3	0	w	1,300	3	3	7	0	150
0	3	4	m	5,500	3	4	0	w-m	3,200
2	2	5	w, w-m	3,900	0	5	2	v, 0	940
2	2	6	0	60	1	1	13	m, w-m	3,600
0	2	8	s, m-s	24,000	3	3	8	w	3,000
1	1	9	v, 0	150	1	5	0	v	390
2	3	0	m, w-m	8,200	0	5	4	0	20

1) James and Brindley, Z. Krist. 78, 470. 1931.

Table V (continuation).

Plane			Observed	Calculated	Plane			Observed	Calculated
h	k	l			h	k	l		
2	2	12	m, w-m	7,400	2	6	0	v	200
0	1	14	0	5	4	4	9	v	680
1	1	14	s	14,000	0	6	8	0	20
2	5	0	v	450	3	6	0	0	140
3	3	9	w	1,100	1	1	8	m, w-m	6,400
0	5	6	0	70	0	1	18	0	100
0	4	10	0	70	0	7	2	w-m	2,700
4	4	0	w-m	3,400	5	5	0	m-s	7,400
4	4	1	w	1,700	5	5	1	v	440
4	4	2	m	9,200	5	5	2	0	160
4	4	3	w-m	3,600	5	5	3	v	1,000
3	5	0	w-m	2,700	1	1	19	v	40
4	4	4	v	780	2	7	0	0	120
0	0	16	m-s	22,000	4	6	0	0	80
4	4	5	0	20	0	7	6	0	50
3	3	11	w, v	900	0	0	20	m-s	11,000
2	2	13	w	900	1	1	20	0	90
2	2	14	v	50	3	7	0	w	1,600
0	3	14	0	400	2	2	19	0	14
0	6	0	0	140	5	6	0	0	160
0	4	12	0	140	0	5	14	v	750
0	6	2	0	60	0	7	10	0	1,100
4	4	6	m, w-m	3,600	1	1	21	0	610
1	6	0	v	1,000	0	8	0	w-m	1,300
3	3	12	w	3,800	6	6	2	m	22,000
4	4	7	v	900					

7. Discussion of the determined Structure.

The excellent agreement of table V may be taken to prove the truth of the initial assumptions, namely the tetragonal grouping of O around S with an oxygen diameter of 2.5 Å, and the octahedral grouping of H_2O around Ni with an H_2O diameter of 2.8 Å.

The water molecules and oxygen atoms belonging to groups on the same rotation axis are in contact with each other, as shewn in figure 3 (where the numbering is that given in § 6). The oxygen atoms 5 touch the water molecules 1, and the oxygen atoms 4 touch the water molecules 2, where the distances are: 5 — 1, 2.72 Å, 4 — 2, 2.72 Å.

The structure also gives that the oxygen atoms 5 touch the water molecules 2 and 3 on neighbouring rotation axes at the same level, and the distances are: 5 — 2, 2.75 Å; 5 — 3, 2.69 Å.

Further the oxygen atoms 4 are close to the water molecules 3 and 1, on rotation axes at different levels. These distances are: 4 — 3, 2.80 Å; 4 — 1, 3.27 Å.

Also the water molecules 1 and 3 on rotation axis at different levels approach to 2.89 Å from each other.
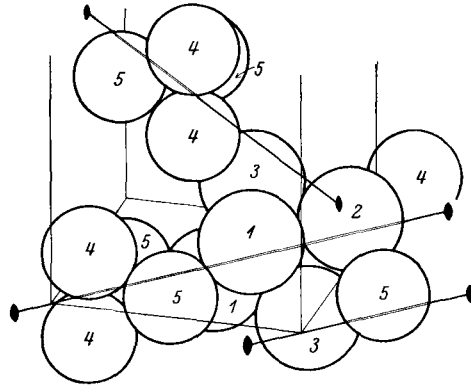

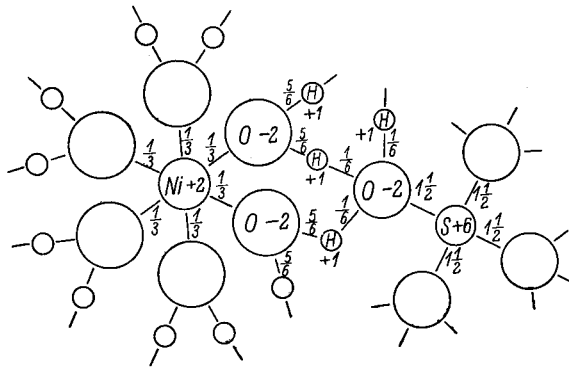Fig. 3. Illustration of the fit of the different groups.

Fig. 4. Diagram of electrostatic bonds.

Each oxygen atom thus touches three water molecules, and each water molecule, two oxygen atoms. The layers parallel to (001) consist of groups closely fitted together, while the different layers fit into each other comparatively badly. This is in no way due to the inaccuracies of analysis; if the parameters are altered to improve the fit between layers the fit within the layers must necessarily be impaired. The atoms build

up into stable layers which must fit into one another as best they can. This is the explanation of the cleavage, and the dominance of the (001) plane.

If we imagine the hydrogen atom of the water molecule to form the link between water and oxygen, then since each oxygen touches three waters and each water two oxygens, the Pauling diagram of electrostatic bonds may easily be constructed, and is shewn in Figure 4.

Owing to the tetrad screw axis perpendicular to (001) it was thought that the crystals should be optically active, and furthermore since there are two possible structures based on the space-groups D_4^t and D_4^8 in which the screw axes have opposite senses, there should be both dextro- and laevo-rotatory crystals. An attempt was made, therefore, to detect this rotation.

It was discovered that the rotation was anomalous; red light suffered a dextro rotation and blue a rather smaller laevo rotation. The magnitudes, however, were not accurately measured, but were of the order of 2° (red) and 1° (blue) per mm. Five small pieces about ½ mm. thick, cleaved from thicker crystals were tried and the rotation due to one of these appeared to be in the opposite sense to that due to the others.
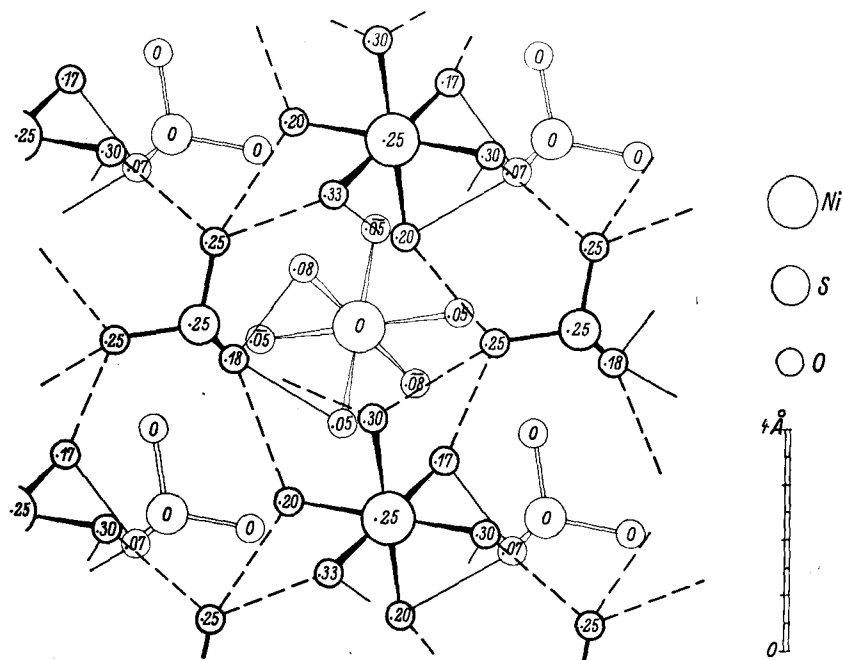

Fig. 5. Projection of structure on (001).

Figure 5 is a diagram of the structure projected on to the (001) plane, and shows sulphate groups and $Ni\,6(H_2O)$ groups at levels 0 and $\frac{1}{4}$. The groups at level $\frac{1}{4}$ are drawn in thick lines, while those at level 0 are drawn in thin lines, and the levels of the various atoms (in fractions of c_0) are indicated by numbers inside the circles. The bonds between the groups at level $\frac{1}{4}$ are shown by thick dotted lines, and the bonds between layers are shown by thin full lines (these bonds are inserted for all the atoms of groups at level $\frac{1}{4}$, excepting for the upper members of the sulphate pairs which coincide in this projection). Each sulphate oxygen may be seen to possess three bonds, and each water oxygen two.

8. Summary.

A structure is proposed for the tetragonal modification of the crystal $NiSO_4 \cdot 6H_2O$. This structure, based on the space group D_4^4 (or its enantiomorph D_4^8), consists of tetrahedral SO_4 groups and octahedral $Ni\,6(H_2O)$ groups, arranged on the dyad axis of the space-group.

Support is given by intensities of reflection estimated from five 30° oscillation photographs.

The structure satisfactorily explains the properties of the crystal, which seems to shew anomalous optical rotation.

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