Die Verbindung La_2CoO_4 ist orthorhombisch deformiert. Die Gitterkonstanten sind

$$a = 5{,}539, \quad b = 12{,}66, \quad c = 5{,}482 \text{ Å}.$$

Für die monokline Pseudozelle, aus der der Zusammenhang mit der tetragonalen Zelle besser hervorgeht, ergibt sich

$$a = c = 3{,}897, \quad b = 12{,}66 \text{ Å} \quad \text{und} \quad \alpha = 90° 36'.$$

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On the structure of anhydrous nickel sulfate.

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Dimaras (1957) recently studied the structure of anhydrous nickel sulphate, establishing an orthorhombic space group *Cmcm*, with $a_0 = 5{\cdot}155$, $b_0 = 7{\cdot}842$, $c_0 = 6{\cdot}338$ Å, $Z = 4$. The equivalent positions for S and O were established on the basis of symmetry and crystal-chemistry configuration considerations, and were finished by trial and error. Table 1 in Dimaras' paper gives

Table 1. *Atomic parameters*

Atoms	Given by Dimaras			Obtained from Fourier projection		
	x	y	z	x	y	z
4 Ni	0	0	0	0	0	0
4 S	0	0·36	¼	0	0·350	¼
8 O_I	0	0·25	0·05	0	0·25	0·02–0·03
8 O_{II}	0·25	0·48	¼	0·25	0·472	¼

experimental values of the structure factors, as well as those calculated from the established atomic positions.

From the observed values given by Dimaras, we have made two Fourier two-dimensional syntheses in order to verify the said positions and, if possible, to refine them, especially for the oxygens. If the method of trial and error is used the relations between O and S should be previously assumed, in so far as it is not possible to adjust independently their parameters. We have taken for the first trials the signs of the structure factors calculated by Dimaras, because of (i) the great difference of atomic numbers between Ni and the other kinds of atoms of the structure, and (ii) the fact that the degree of freedom for the S atoms is only one, if symmetry considerations are taken into account, and hence, the F's mostly remain unchanged in signs.

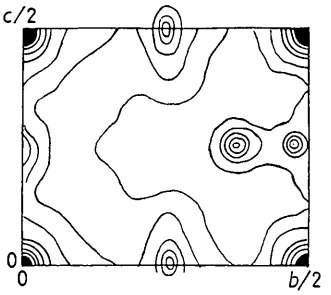

Fig. 1. Fourier projection of $NiSO_4$ on (100). Contours are drawn at equal intervals on an arbitrary scale.

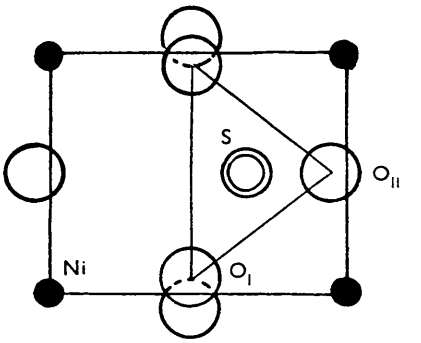

Fig. 2. Structure projection of $NiSO_4$ on (100).

First we made the *pmm* projection on to the plane (010), but we did not obtain sufficiently good results on the positions of the atoms, owing to the fact that only a few terms were available, and hence the Fourier synthesis would not resolve.

On the contrary, the *pgm* projection on to the plane (100) led to good convergence after having made a linear synthesis along the b axis which enabled us to determine an adequate temperature-convergence factor. Once this factor was introduced we made the two-dimensional synthesis $\sum_k \sum_l$. Fig. 1 shows the Fourier projection whilst Fig. 2 shows the corresponding structure projection. The positions of the oxygens $O_I(x = 0, y = 0{\cdot}25)$ along the c axis cannot be definitely established because of the superposition of densities with a symmetry line normal to the c axis. Nevertheless, it seems to be reasonable to assign a value $z = 0{\cdot}02$–$0{\cdot}03$ rather than 0·05. On the contrary, in the case of O_{II}, the positions appear very sharply, and give for the corresponding parameter a value $y = 0{\cdot}472$. In the case of S, $y = 0{\cdot}350$. The structure obviously agrees with that proposed by Dimaras, with small differences in the parameters, as is shown in Table 1.

The errors in the parameter values thus established are mainly due to the error of the observed structure factors themselves.

We are indebted to Miss Hebe Paolo for having kindly collaborated during the calculations.

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