tensities were less than 1% and, with the exception of the *h*00 and *hhh* reflexions, at least six symmetry-equivalent reflexions were measured, the final observed structure factors being taken to be the average over their symmetry equivalents. All reflexions having $\sin\theta < 70°$ were measured for planes of even indices but, for planes of odd indices, only reflexions having $\sin\theta < 54°$ could be measured to the desired accuracy in an acceptable time due to the low reflectivity.

Since magnesium oxide has the rock-salt structure, the thermal parameters for the two ions can be found by simple graphical methods. Only those reflexions having $(\sin\theta)/\lambda > 0·35$ were used since the corresponding scattering factors are then almost independent of the state of ionization of the atoms and lower-order reflexions may be suffering from extinction. The scattering factors used were those in *International Tables for X-ray Crystallography* (1968). The temperature factors obtained were:

$$B(\text{magnesium}) = 0·30 \pm 0·01 \text{ Å}^2$$
$$B(\text{oxygen}) = 0·34 \pm 0·02 \text{ Å}^2.$$

These values are considerably higher than those obtained by Togawa which were calculated using only those reflexions in the region $(\sin\theta)/\lambda < 0·63$, the calculated structure factor in this range being dependent on the state of ionization of the magnesium and oxygen ions.

Table 1 shows the observed and calculated structure factors for magnesium oxide. The *R* index is 0·0062, showing an agreement between the observed and calculated structure factor comparable with that obtained with similar materials using data measured on the same diffractometer (*e.g.* Killean, Lawrence & Sharma, 1972).

Table 1. *Observed and calculated structure factors*

h	*k*	*l*	F_o	F_c
4	4	0	29·22	29·00
6	0	0	16·75	16·70
4	4	2	16·55	16·70
6	2	0	15·54	15·51
6	2	2	14·52	14·34
4	4	4	13·38	13·41
6	4	0	12·68	12·63
6	4	2	11·92	11·89
8	0	0	10·90	10·73
8	2	0	10·25	10·21
6	4	4	10·23	10·21
6	6	0	9·84	9·74
8	2	2	9·79	9·74
6	6	2	9·38	9·36
8	4	0	9·06	8·99
8	4	2	8·61	8·62
6	6	4	8·28	8·29
8	4	4	7·61	7·69
10	0	0	7·30	7·41
8	6	0	7·37	7·41
10	2	0	7·07	7·15
8	6	2	7·14	7·15
10	2	2	6·92	6·91
6	6	6	6·86	6·91
10	4	0	6·49	6·48
8	6	4	6·52	6·48
10	4	2	6·21	6·27
3	3	3	7·19	7·23
5	1	1	7·23	7·23
5	3	1	5·46	5·47
5	3	3	4·15	4·23
7	1	1	3·30	3·33
5	5	1	3·32	3·33
7	3	1	2·68	2·67
5	5	3	2·65	2·67
7	3	3	2·19	2·22
7	5	1	1·94	1·91
5	5	5	1·95	1·91
9	1	1	1·68	1·67
7	5	3	1·64	1·67

References

International Tables for X-ray Crystallography (1968). Vol. III. p. 202. Birmingham: Kynoch Press.

Killean, R. C. G., Lawrence, J. L. & Sharma, V. C. (1972). *Acta Cryst.* **A28**, 405–407.

Lawrence, J. L. (1972). *Acta Cryst.* **A28**, 400–404.

Togawa, S. (1965). *J. Phys. Soc. Japan.* **20**, 742–752.

Acta Cryst. (1973) **A29**, 96

Constrained refinement techniques applied to the structure of ammonium hydrogen sulphate above the ferroelectric transition: errata.

By R. J. Nelmes, *Department of Physics, University of Edinburgh, The King's Buildings, Mayfield Road, Edinburgh EH9 3JZ, Scotland*

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Corrections are given to *Acta Cryst.* (1972), **A28**, 445–454.

Three printing errors have been found in Nelmes (1972). The corrections are as follows:

(1) In Table 6, for atom O(1)$^-$ *Z* should be 2·435 and not 2·345.

(2) In Table 6, for atom O(7) U_{31} should be $-0·0171$ and not $-0·171$.

(3) In the heading of Table 7, after the colon on the third line, the correct form is ' **T** parameters (in order T_{11}, T_{22}, T_{33}, T_{23}, T_{31}, T_{12}) . . .', *i.e.* T_{33} and T_{23} have been interchanged.

Reference

Nelmes, R. J. (1972). *Acta Cryst.* **A28**, 445-454.