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The crystal structure of $(+)_{589}$-tris-[(−)-*trans*-1,2-diaminocyclohexane]cobalt(III) chloride monohydrate (*'ob'*isomer). Corrigenda.

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The atomic parameters of O(1) in the paper by Kobayashi, Marumo & Saito [*Acta Cryst.* (1972). B28, 2709–2715] are incorrect and the last line of Table 2(*a*) should read O(1) 2968 (6) 4991 (13) 7042 (10) 94 (6) 194 (11) 254 (16) 40 (12) 90 (8) 9 (20).

An incorrect population factor was used for O(1) in our recent paper on the crystal structure of

$$(+)_{589}\text{-}[Co(\text{-chxn})_3]Cl_3 . H_2O$$

(Kobayashi, Marumo & Saito, 1972). The oxygen atoms are randomly distributed on the fourfold general position with population of 0·5. The last line in Table 2(*a*) should read as in the above abstract.

There is no significant change in the positional and thermal parameters of the other atoms. The final R value is 0·031.

Reference

KOBAYASHI, A., MARUMO, F. & SAITO, Y. (1972). *Acta Cryst.* B28, 2709–2715.

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The structures of fluorides. V. The x-parameter in NiF_2.

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A least-squares refinement with 22 integrated intensities from a neutron powder pattern of NiF_2 gave an unweighted R index on F^2 of 3·5% and a fluorine x parameter 0·3052 (6). The octahedron was found to be undistorted, confirming that rutile-type fluorides as well as oxides cannot be completely described by a simple Born model.

The observed distortions of octahedra found in rutile-type AB_2 oxides and fluorides are of interest because of their correlation with theoretical predictions. These distortions can be expressed in terms of the difference between the lengths of the 4 coplanar bonds (l_1) located in the (110) plane and the 2 axial bonds (l_2) normal to (110). A Born model predicts $l_1 > l_2$. Baur & Khan (1971) found with X-ray diffraction that, while CrO_2, RuO_2, SnO_2, OsO_2, PbO_2, MgF_2, MnF_2, FeF_2, CoF_2, NiF_2 and ZnF_2 have $l_1 > l_2$, SiO_2, TiO_2 and GeO_2 have $l_1 < l_2$. In view of this, they pointed out that the Born model was probably inadequate. Jahn–Teller distortions are only likely in FeF_2 (Knox, 1961).

While studying fluorides present in fluorine generators, we measured the x_F parameter of NiF_2 at 21 °C by powder neutron diffraction. This technique does not have the problems of absorption and extinction encountered in the X-ray method. Pure NiF_2 was prepared by heating $NiCl_2$ in F_2 at 275 °C in a flow reactor (Brauer, 1963), and removing absorbed F_2 (Watanabe & Takashima, 1971) by pumping. The pattern was collected on HIFAR, the AAEC research reactor, by the elastic diffraction technique (Cagliotti, 1970) with $\lambda = 1{\cdot}075$ Å. x_F, B_{Ni}, and B_F where B is the isotropic Debye–Waller factor, were determined by a least-squares refinement of 22 integrated intensities, the function minimized being $\sum_i [w_i(\sum_j JF_o^2 - \sum_j JF_c^2)^2]$, where i is a peak with j components each with multiplicity J.

The final discrepancy index, $R = \sum_i (\sum JF_o^2 - \sum JF_c^2)/$

Table 1. *Observed and calculated integrated intensities in the neutron powder pattern of* NiF_2 *at* 21 °C

hkl	$\sum JF_o^2$	$\sum JF_c^2$	σ
110	21·1	21·0	0·4
101	12·5	13·4	0·4
020	0·3	0·6	0·3
111	29·3	28·7	0·6
120	11·6	13·1	0·5
121	103·1	102·6	1·5
220	39·6	41·3	1·1
002	33·1	32·6	1·2
130	15·1	14·6	1·0
221	5·9	5·7	0·9
112 } 031	151·6	148·0	2·3
131	15·5	15·0	1·3
230 } 022	4·9	4·5	1·1
122	24·9	23·3	1·4
231	5·1	5·4	1·1
040	21·4	20·4	1·6
140 } 222	102·3	101·0	2·5
330	42·1	44·4	1·9
132 } 141	72·7	75·6	2·5
240 } 331	24·5	22·1	1·9
103	12·7	11·4	1·7
232 } 241 } 113	48·1	51·6	2·3