Erratum

Transition Metal Iodates. VII. Crystallographic and Nonlinear Optic Survey of the 4*f*-lodates

S. C. ABRAHAMS, J. L. BERNSTEIN, AND K. NASSAU

Bell Laboratories, Murray Hill, New Jersey 07974

Received May 14, 1977

Several interpretive and typographic errors have been found in paper VII of this series (1) with the above title.

Table II (1). Gd(IO₃)₃ spacings obtained (2) with a Guinier-Hägg focusing camera give lattice constants $a = 13.4365 \pm 9$, b = 8.5226 ± 5 , $c = 7.1356 \pm 5$ Å, $\beta = 99.717 \pm 0.007^{\circ}$ at 297°K (each translation is about 0.35% larger than that given in Table I (1)). The Miller indices 003, 521, and 332 for Gd(IO₃)₃ should hence be 203, 512, and 023; it is possible that other index assignments in Table II (1) will change as more accurate spacings become available. The value of d_{obs} (021) for Gd(IO₃)₃ should read 3.632 Å, and I(310) and I(202) for Tb(IO₃)₃ should be 1 and 3, respectively.

Table IV (1). The Miller index 201 should be $\overline{2}11$ and d_{calc} ($\overline{2}11$) for Yb(IO₃)₃ should be 3.49 Å; d_{calc} (015) for Lu(IO₃)₃ should read 2.71 Å.

Table V (1). The observed but unindexed d-spacings and intensities given for "Ce(IO₃)₃, Type V" are now assigned to Ce(IO₃)₃ · H₂O,

TABLE VIA

OBSERVED AND CALCULATED <i>d</i> -Spacings and	OBSERVED	INTENSITIES OF	La and	Ce(IO ₃),	· H	,0
--	----------	----------------	--------	-----------------------	-----	----

	$La(IO_3)_3 \cdot \frac{1}{2}H_2O$			Ce(IO ₃) ₃ · ½H ₂ O		
h k l	$d_{\rm obs}$ (Å)	$d_{\rm calc}({\rm \dot{A}})$	I	$d_{\rm obs}$ (Å)	d _{calc} (Å)	I
111	4.83	4.81	1	4.82	4.80	1
211	4.39	4.39	5	4.37	4.39	3
410	3.97	3.94	6	3.96	3.95	5
401	3.86	3.83	2	3.84	3.84	5
020	3.70	3.69	1	3.69	3.69	1
120	3.62	3.62	4	3.62	3.62	3
220	3.44	3.43	3	3.43	3.43	3
002	3.38	3.37	1	3.37	3.36	3
102	3.31	3.31	10	3.30	3.31	9
501	3.26	3.26	6	3.25	3.27	5
021	3.22	3.24	6	3.23	3.23	5
202	3.16	3.17	7	3.16	3.16	6
221	3.05	3.06	9	3.04	3.06	10
112	3.02	3.02	1			_
302	_			2.96	2.96	1

Copyright © 1977 by Academic Press, Inc. All rights of reproduction in any form reserved. Printed in Great Britain.

 $\begin{array}{c} CRYSTALLOGRAPHIC DATA FOR LA AND \\ Ce(IO_3)_3 \cdot \frac{1}{2}H_2O^a \\ \hline \\ \hline \\ La(IO_3)_3 \cdot \frac{1}{2}H_2O & Ce(IO_3)_3 \cdot \frac{1}{2}H_2O \\ \hline \\ a(\dot{A}) & 18.61 \pm 6 & 18.73 \pm 4 \\ b(\dot{A}) & 7.39 \pm 1 & 7.38 \pm 1 \\ c(\dot{A}) & 6.74 \pm 1 & 6.72 \pm 1 \\ \hline \end{array}$

926.60

P2,2,2,

 4.7 ± 0.2

4.82

4

TABLE VIB

^a From Table VIA data, by least-squares refinement.

928.48

P2,2,2,

4.81

4

Type II, and are indexed as in the new Table VIIA, given below.

Table VI (1). The assigned Miller indices are inconsistent with the space group $C222_1$ of Table VII (1) but the observed spacings may be indexed with the primitive space group $P2_12_12_12_1$ as given in the new Table VIA. The crystallographic data corresponding to this new Table are presented, for La(IO₃)₃ $\cdot \frac{1}{2}H_2O$ and Ce(IO₃)₃ $\cdot \frac{1}{2}H_2O$, in the new Table VIB. Repeated attempts to grow and isolate additional single crystals of these two hemihydrates were unsuccessful.

Table VII (1). The data given for $La(IO_3)_3 \cdot \frac{1}{2}H_2O$ should be replaced by those in new Table VIB, based on the spacings of new Table VIA.

TABLE VIIA

Observed d-Spacings and Intensities of $Ce(IO_3)_3 \cdot H_2O$, Type II

hkl	d _{obs} (Å)	d _{calc} (Å)	I
310	4.85	4.85	4
020	3.70	3.71	6
002	3.32	3.36	10
202	3.18	3.17	1
112	3.02	3.02	8
402	2.75	2.75	1
530	2.08	2.08	1
531	1.99	1.99	2
912	1.75	1.74	2
404	1.57	1.59	1

TABLE VIIB

Crystallograp Ce(IO ₃) ₃ · H	hic Data for 20, Type IIª
a (Å)	19.20 ± 3
b (Å)	7.42 ± 1
c (Å)	6.72 ± 1
Volume (Å ³)	957.4
S.G.	C2221
$Dx (g \text{ cm}^{-3})$	4.74
<i>Dm</i> (g cm ⁻³)	
Z	4

^a From Table VIIA data, by least-squares refinement.

monohydrate Α second phase, Ce- $(IO_3)_3 \cdot H_2O$, Type II, previously (1) identified as " $Ce(IO_3)_3$, Type V," is formed by spontaneous hydration on exposure to the atmosphere of the anhydride produced by dehydration of amorphous $Ce(IO_3)_1$ (3). The d-spacings of this compound are given in new Table VIIA with Miller indices assigned on the basis of the crystallographic data in new Table VIIB. A single crystal, now thought to be the nearly stoichiometric $Ce(IO_3)_3 \cdot H_2O$, Type II, gave lattice constants close to those of new Table VIIB; this was previously reported in Table VII (1) under the designation "Ce(IO₃)₃ $\cdot \frac{1}{2}$ H₂O." Further attempts to isolate additional single crystals of $Ce(IO_3)_1 \cdot H_2O_1$ Type II were unsuccessful and confirming analyses could not be undertaken since no previously prepared material remained available.

The designation of the "Type 1" monohydrates in paper VI of this series (3) should now be changed to "Type 1_t ," and the designation "Ce(IO₃)₃, Type V" changed to "Ce(IO₃)₃ · H₂O, Type 1_{1t} ."

It is a pleasure to thank S. Weissmann and R. Liminga for drawing our attention to some of the above errors.

References

- I. S. C. ABRAHAMS, J. L. BERNSTEIN AND K. NASSAU, J. Solid State Chem. 16, 173 (1976).
- R. LIMINGA, S. C. ABRAHAMS, AND J. L. BERNSTEIN. J. Chem. Phys. 67 (1977).
- 3. K. NASSAU, J. W. SHIEVER, AND B. E. PRESCOTT, J. Solid State Chem. 14, 122 (1975).

Volume (Å³)

 $Dx (g cm^{-3})$

 $Dm (g cm^{-3})$

\$.G.

Ζ