



Fig. 1. Monoclinic cell parameters (Å) of RE NbO<sub>4</sub> and ionic radii of the corresponding eight-coordinated trivalent rare earth (after Shannon & Prewitt, 1969, 1970).

in oxides. The contraction of the rare earths' radii is essentially linear, except for positive deviations at La and Lu. This deviation from linearity is reflected in the cell parameters of the RE NbO<sub>4</sub> compounds.

The help of William Holt who prepared several of the compounds, and Clarence Gooden who assisted with the data refinement, is acknowledged.

#### References

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Table 2. X-ray powder pattern of TmNbO<sub>4</sub>

$d_{\text{obs}}$	$d_{\text{calc}}$	$I/I_0$	$hkl$
5.44	5.44	2	020
4.718	4.720	2	110
4.562	4.563	9	011
3.106	3.105	100	$\bar{1}21$
2.981	2.980	10	130
2.939	2.939	90	031, 121
2.718	2.717	20	040
2.620	2.621	20	200
2.514	2.513	25	002
2.285	2.286	2	$\bar{1}12$ , 022
2.206	2.205	7	$\bar{1}41$ , 211
2.145	2.144	7	141
2.005	2.006	2	150, $\bar{2}31$
1.996	1.996	9	051
1.966	1.966	3	$\bar{1}32$
1.891	1.891	3	$\bar{2}02$
1.8865	1.8867	40	240
1.8455	1.8458	30	042
1.7457	1.7460	12	202
1.6564	1.6562	2	013
1.6344	1.6343	16	$\bar{1}03$ , $\bar{1}61$
1.6161	1.6163	14	$\bar{3}21$
1.6083	1.6086	24	161
1.5737	1.5735	2	330
1.5654	1.5657	13	$\bar{1}23$
1.5524	1.5526	9	$\bar{2}42$
1.5444	1.5441	13	152, $\bar{3}21$
1.4999	1.5000	11	123

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**Note on the space group of potassium hydrogeniodate(V), KIO<sub>3</sub>.HIO<sub>3</sub>. A correction.** By G. KEMPER and AAFJE VOS, *Laboratorium voor Structuurchemie, Rijksuniversiteit Groningen, Zernikelaan, Paddepoel, Groningen, The Netherlands*

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Contrary to the conclusion given in an earlier note, we have adopted the space group  $P2_1/c$  for KIO<sub>3</sub>.HIO<sub>3</sub>, as the observed piezoelectric effect appeared to be caused by a thin layer of KIO<sub>3</sub> present on the surface of the crystal of KIO<sub>3</sub>.HIO<sub>3</sub> used for the piezoelectricity measurement.

The difficulties concerning the space group of KIO<sub>3</sub>.HIO<sub>3</sub> reported in an earlier note (Kemper & Vos, 1970) have now been solved. It appeared that the piezoelectric effect which had been measured for a large crystal of KIO<sub>3</sub>.HIO<sub>3</sub> having a volume of approximately 0.25 mm<sup>3</sup>, is caused by a thin layer of KIO<sub>3</sub> deposited on the surface of the crystal. The presence of the KIO<sub>3</sub> layer was found by a careful study of a zero level Weissenberg photograph about the  $b$  axis of the large crystal, taken with Ni-filtered Cu radiation. This

photograph showed 13 weak streaks which were identified as KIO<sub>3</sub> reflexions by their good fit to the pattern of a zero-layer Weissenberg photograph of the room temperature modification of KIO<sub>3</sub> at present being studied by F. van Bolhuis in our laboratory. We have therefore adopted  $P2_1/c$  as the correct space group for KIO<sub>3</sub>.HIO<sub>3</sub> in agreement with the results of the X-ray refinement reported in the earlier note (Kemper & Vos, 1970). In the mean time a neutron powder-diffraction study of KIO<sub>3</sub>.HIO<sub>3</sub> and of KIO<sub>3</sub>.DIO<sub>3</sub>

carried out by Dr H. M. Rietveld at the Reactor Centrum Nederland, Petten (N.H.), has shown that the hydrogen (deuterium) atoms also obey the symmetry P21/c.

The crystal structure of KIO3.HIO3 has recently also been determined by Chan & Einstein (1971). In view of the discussion of the piezoelectric effect given above, it is reasonable to assume that the strong second harmonic effect reported for KIO3.HIO3 by these authors is due to the presence of KIO3 (or HIO3) on the surface of the crystals.

A full account of our work and a comparison with the structure of KIO3.HIO3 described in space group P21/c by Chan & Einstein will be published in the Canadian Journal of Chemistry.

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A redetermination of the crystal structure of tetramethyldiphosphine disulphide. By J. D. LEE and G. W. GOODACRE, Department of Chemistry, University of Technology, Loughborough, Leicestershire, England

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The correct structure factor table to an earlier paper [Acta Cryst. (1971) B27, 302] is given.

In an earlier paper of the above title (Lee & Goodacre, 1971) the two parts of the structure factor table printed (Table 4, page 305) are identical. The whole Table should be replaced by that given here.

Table 4. Observed and calculated structure factors

Table with 10 columns: h, k, l, Fo, Fc, h, k, l, Fo, Fc. Contains observed and calculated structure factor data for tetramethyldiphosphine disulphide.

Table 4 (cont.)

Continuation of Table 4 with 10 columns: h, k, l, Fo, Fc, h, k, l, Fo, Fc. Contains observed and calculated structure factor data.

Reference

LEE, J. D. & GOODACRE, G. W. (1971). Acta Cryst. B27, 302.