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Unit cell and space group of $2Nb_2O_5.Ta_2O_5$.

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In a recent study of the Nb_2O_5–Ta_2O_5 system, Holtzberg & Reisman (1961) reported the compound $2Nb_2O_5.Ta_2O_5$, and on the basis of its powder data gave the unit cell as body centered cubic with $a = 15{\cdot}76$ Å. The existence of this compound was currently confirmed in our laboratory as part of a detailed study of the equilibria in the binary system Nb_2O_5–Ta_2O_5. This note reports the results of the powder and single crystal studies of the compound.

Single crystals of the compound were grown by annealing powder compacts of Nb_2O_5 and Ta_2O_5 mixtures at 1400 °C. for four weeks in air. Both microscopic observations and X-ray measurements confirmed that the needle shaped crystals which formed during the annealing treatment increased in proportion as the sample composition approached the ideal 2:1 ratio, and at this composition, the sample consisted essentially of these crystals.

Using the precession method, diffraction studies of the single crystals chosen from a Nb_2O_5–32% Ta_2O_5 sample established unequivocally the unit cell as body centered tetragonal rather than cubic as reported by Holtzberg & Reisman (1961). The cell dimensions are:

$$a = 15{\cdot}77 \pm 0{\cdot}01,\ c = 3{\cdot}84 \pm 0{\cdot}01 \text{ Å}.$$

The single crystals because of their extremely small size ($\sim 7 \times 30\mu$) were unsuitable for density measurements; loose powder samples were used instead, and an approximate value of 6·10 g.cm.$^{-3}$ corresponding to 4 formula weights per unit cell (cal. den. 6·76) was obtained. From the diffraction symmetry and systematic absences, the possible space group is $I4$, $I\bar{4}$, or $I4/m$. Table 1 lists the first 20 powder pattern reflections, the observed relative intensities and the corresponding interplanar spacings showing the agreement between the calculated and observed values.

Table 1. *Powder pattern data*

hkl	d_c	d_o	Rel. int.
200	7·887 Å	7·89 Å	5
220	5·577	5·574	9
310	4·989	4·997	25
400	3·943	3·953	5
330	3·719	3·724	21
101	3·730		
240	3·528	3·535	100
121	3·372	3·370	6
150	3·094	3·100	5
301	3·101		
231	2·883	2·884	11
350	2·706	2·711	13
141	2·710		
600	2·629	2·633	4
260	2·494	2·498	24
501, 341	2·438	2·442	5
521	2·329	2·327	5
170, 550	2·231	2·233	4
460	2·187	2·192	5
161	2·148	2·149	3
370	2·071	2·074	27
451	2·073		
361	2·005	2·003	3
800	1·971	1·975	6

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Reference

HOLTZBERG, F. & REISMAN, A. (1961). *J. Phys. Chem.* **65**, 1192.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (D. W. Smits, Mathematisch Instituut, University of Groningen, Reitdiepskade 4, Groningen, The Netherlands).

IUCr World List of Crystallographic Computer Programs*

The first edition (September 1962) of the IUCr World List of Crystallographic Computer Programs, compiled under the auspices of the Commission on Crystallographic Computing of the International Union of Crystallography, is distributed with the current (November 1962) issue of Acta Crystallographica. The list is similar in format to that previously published by the American Crystallographic Association (ACA). The format is based on IBM punched cards. Each computer program is represented by a *title card* containing essential information concerning the program (machinetype, function of program, names of programmers, availability of program and operating instructions, etc.) in highly compressed form, followed optionally by one or more *abstract cards* with additional information. The main body of the list consists of a tabulator listing of these cards, sorted according to machinetype and function. An author programmer index (with mailing addresses), a list of abbreviations, an accession-number index for aid in cross-referencing, and a detailed description of the format are also printed from punched cards as accessories to the list. The present World List contains entries for 577 programs, many of which also appear in the ACA lists. Nearly all programs listed were in existence prior to 1 January 1962.

Additional copies of the List, subject to limited supply, are available from the Editor, D. P. Shoemaker (Massachusetts Institute of Technology, Cambridge 39, Mass., U.S.A.), from the Chairman of the Commission, G. A. Jeffrey (Crystallographic Laboratory, University of Pittsburgh, Pittsburgh, Pa., U.S.A.), or from the General Secretary of the Union, D. W. Smits (Mathematisch Instituut, Reitdiepskade 4, Groningen, The Netherlands).

* See also *Acta Cryst.*, **14**, 898 (1961).