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The crystal structure of bistetramethylammonium dioxotetrabromouranate(VI).*

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Crystals of $[(CH_3)_4N]_2UO_2Br_4$ are tetragonal; the space group is $P4_2/mnm$ with $a=9{\cdot}35$, $c=11{\cdot}68$ Å, and $Z=2$. The uranium–oxygen bond distance is 1·72 Å.

The infrared-active stretching frequency of the linear $(O–U–O)^{2+}$ group has been used to determine bond properties of this group in the presence of various ligands about the uranium atom (Hoekstra, 1963). The relationship is given by $R=\beta F_{U-O}^{-1/3}+d_{U-O}$, where F_{U-O} represents the force constant for the infrared-active stretching mode of the O–U–O group and β and d_{U-O} are constants. A single-crystal X-ray diffraction structure determination of bistetramethylammonium dioxotetrabromouranate(VI) was undertaken to test the relationship between the infrared stretching frequency of the uranyl group and the uranium–oxygen bond distance in a compound in which the other ligands are heavy by comparison with oxygen.

The title compound was prepared by reducing $UO_2(OAc)_2$ in a Jones Reductor, adding $(CH_3)_4NBr$, and precipitating the product from an ethanol–acetone mixture. The product was recrystallized from a concentrated HBr–ethanol solution. Lattice constants for the tetragonal unit cell, $a=9{\cdot}35$ (1) and $c=11{\cdot}68$ (1) Å, were determined from powder diffractometer data using NaCl as a calibration, $a=5{\cdot}64056$ Å (Wyckoff, 1965). Estimated errors are in parentheses. The observed density (2·40 g cm^{-3}) measured using the flotation method with a solvent mixture of carbon tetrachloride and tetrabromoethane agrees with the calculated density assuming two molecules per unit cell (2·40 g cm^{-3}).

A wedge-shaped crystal approximately 0·15 × 0·16 × 0·15 mm was used for intensity measurements. A total of 504 independent reflections were measured by the θ–2θ scan technique using a computer-controlled, automatic diffractometer. Of these, 395 were observed greater than $2{\cdot}5\sigma$. Zirconium-filtered molybdenum radiation ($\lambda=0{\cdot}7107$ Å) was used. No corrections for absorption ($\mu=184{\cdot}1$ cm^{-1}) or extinction were included. Atomic scattering factors were those given by Cromer (1968); anomalous dispersion corrections were applied to uranium and bromine. Systematic absences were determined from a rapid peak-top counting procedure. Extinctions were noted for $0kl$ with $k+l$ odd, which is consistent with space groups $P4_2/mnm$, $P4n2$, and $P4_2nm$. The choice of $P4_2mnm$ is confirmed by the final structure results.

Uranium and bromine atom positions were obtained from a Patterson synthesis; all other non-hydrogen atoms were located and refined by Fourier and least-squares methods. Because hydrogen atoms could not be unambiguously located from the last difference map, they were not included in these calculations. A weighting scheme based on counter statistics (Stout & Jensen, 1968) was applied. The final weighted residual

$$R_w=\left(\frac{\sum |W_i|F_o|-W_i|F_c||}{\sum W_i|F_o|}\right)$$

was 0·063. All parameter changes were less than $0{\cdot}2\sigma$ for the respective parameters. Positional and thermal parameters are shown in Table 1.†

The uranium complex is octahedral with a bromine atom above and one below the uranium atom in the direction of the c axis. The other two bromine atoms and the two oxygen atoms lie in a plane perpendicular to this direction. Bond angles about the uranium atom are restricted by the site symmetry to those of a regular octahedron. Tetramethylammonium cations are tetrahedral. Important interatomic distances are U–O = 1·72 (2) Å; U–Br = 2·793 (5) Å along

Table 1. *Positional and thermal parameters for* $[(CH_3)_4N]_2UO_2Br_4$

Standard deviations, in parentheses, are for the last figure of the parameter listed.
Anisotropic temperature factors are expressed as $\exp\left[-\frac{1}{4}(B_{11}h^2a^{*2}+\ldots+2B_{12}hka^*b^*+\ldots)\right]$.

	Wyckoff numbers	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{23}	B_{13}
U	$2a$	0	0	0	3·33 (9)	B_{11}	4·3 (2)	0·2 (2)	0	0
Br(1)	$4e$	0	0	0·2391 (4)	6·0 (2)	B_{11}	4·5 (3)	−0·6 (4)	0	0
Br(2)	$4f$	0·2137 (4)	x	0	4·2 (2)	B_{11}	5·8 (3)	−0·2 (2)	0	0
O	$4g$	0·130 (2)	$-x$	0	2·2 (9)	B_{11}	4 (2)	−2 (1)	0	0
N	$4d$	$\frac{1}{2}$	1	$\frac{1}{4}$	5 (1)	B_{11}	5 (2)	0	0	0
C	$16k$	0·422 (3)	0·892 (3)	0·175 (2)	8 (2)	5 (2)	6 (2)	−2 (1)	−2 (1)	−2 (2)

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† The structure-factor list has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 30269 (2 pp.). Copies may be obtained through the Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

[001], and U–Br = 2·826 (6) Å in the perpendicular plane; and C–N = 1·52 (3) Å.

The infrared spectrum of the uranium complex using a KBr matrix contains a peak with a maximum at 895 cm^{-1} that can be assigned to the asymmetric stretching vibration of the $(O–U–O)^{2+}$ group. By using 1·08 and 1·17 for the values of the constants β and d_{U-O} respectively the U–O bond distance is calculated to be 1·73 Å in good agreement with the distance found by X-ray diffraction. Bond distances for this compound are in good agreement with those found for $Cs_2UO_2Br_4$ (Mikhailov & Kuznetsov, 1971).

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International Union of Crystallography

Tenth General Assembly and International Congress of Crystallography

By invitation of the Fundamenteel Onderzoek der Materie met Röntgen en Elektronenstralen (FOMRE), the Tenth General Assembly and International Congress of Crystallography will be held in Amsterdam, The Netherlands, 7–15 August 1975.

The arrangement of the scientific programme will in general be similar to that of the Ninth Congress held in Japan in 1972. There will be General Lectures, Scientific Sessions on topics of interest for today's crystallography and chemistry, Poster Sessions, Open Sessions of Commissions of the Union and *ad hoc* meetings. Participants will be invited to submit abstracts of recent work on crystallographic subjects. Upon acceptance, these contributions will be printed in the book of abstracts of the Congress. For oral presentation in the formal scientific sessions or for the Poster Sessions, a selection will be made from the papers lying within the range of the congress topics. The *ad hoc* meetings are intended mainly to encourage free discussion.

A commercial exhibition will be organized in which manufacturers and distributors of equipment related to crystallographic research may display their products. Further information can be obtained from the Organizing Committee. For the accompanying members, a choice of tours will be offered. The details of this programme and the social programme will be published in the *First Circular*.

Professor D. Feil is Chairman of the Organizing Committee and Dr H. M. Rietveld is Secretary and Treasurer. Correspondence should be addressed to:

The Organizing Committee
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Further details of the General Assembly and Congress, including arrangements for registration, accommodation, scientific visits, *etc.*, will be published in the *First Circular*, which will be distributed in the second half of 1974. Persons interested in receiving the *First Circular* are requested to complete an application card and return it to the Organizing Committee before 1 June 1974. Application cards may be obtained from the secretaries of the National Committees for Crystallography or from the Organizing Committee. Please bring this announcement to the notice of your colleagues.

International Union of Crystallography Commission on Crystallographic Computing

Call for material for supplement to the third edition of the *World List of Crystallographic Computer Programs*

The third edition of the *World List of Crystallographic Computer Programs* has been published in the *Journal of Applied Crystallography* (1973), part 4, pp. 309–346. The required information for submission of programs to this list was first described in an announcement in *Acta Cryst.* (1971), part 4, pp. 393–396, and again as part of the *World List*.

Since a large number of useful crystallographic computer programs were not included in the third edition, the Commission on Crystallographic Computing has decided to publish supplements to the list on an annual basis, until such time as a completely new list is required. This work is done for the benefit of crystallographers in general, and to avoid any wasteful duplication of effort. Therefore, the Commission wishes to take this opportunity to urge all crystallographer programmers to take the time to prepare the material required for the proposed supplement. The formats and abbreviations will be identical with those for the third edition. Please send the necessary information about your unlisted programs, within two months from the date of publication of this announcement, to the Editor in charge of the Supplement: Dr G. C. Bassi, CNRS Laboratoire de Rayons X, B.P. No. 166, Centre de Tri, 38042 Grenoble-Cedex, France.