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THE CRYSTAL STRUCTURE OF THORIUM NITRATE

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November 20, 1950

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Carbide & Carbon Chemicals Division (K-25 Plant)	20-23
Chief of Naval Research	24
Dow Chemical Company	25
General Electric Company, Richland	26-31
Hanford Operations Office	32
Idaho Operations Office	33-36
Iowa State College	37
Kellex Corporation	38
Knolls Atomic Power Laboratory	39-42
Los Alamos	43-45
Mallinckrodt Chemical Works	46
Massachusetts Institute of Technology (Gaudin)	47
Massachusetts Institute of Technology (Kaufmann)	48
Mound Laboratory	49-51
National Advisory Committee for Aeronautics	52
National Bureau of Standards	53
Naval Medical Research Institute	54
Naval Radiological Defense Laboratory	55
Naval Research Laboratory	56
NEPA Project	57-59
New Brunswick Laboratory	60
New York Operations Office	61-62
North American Aviation, Inc.	63
Oak Ridge National Laboratory, X-10 Site	64-71
Oak Ridge National Laboratory, Y-12 Site	72-75
Patent Branch, Washington	76
Sylvania Electric Products, Inc.	77
Technical Information Service, Oak Ridge	78-92
UCLA Medical Research Laboratory (Warren)	93
U. S. Geological Survey	94
University of California Radiation Laboratory	95-98
University of Rochester	99-100
Western Reserve University (Friedell)	101
Westinghouse Electric Corporation	102-103
Total	103

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THE CRYSTAL STRUCTURE OF THORIUM NITRATE

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November 20, 1950

ABSTRACT

Thorium nitrate, $Th(NO_3)_4 \cdot 6H_2O$ is orthorhombic with

$$\underline{a} = 11.2 \text{ Å}$$

$$\underline{b} = 22.8$$

$$\underline{c} = 10.6$$

The space group is Fdd -- C_{2v}^{19} and there are eight molecules in the unit cell. Only the unit cell and thorium positions have been determined.

THE CRYSTAL STRUCTURE OF THORIUM NITRATE

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Studies were made of single crystals of thorium nitrate hydrate which we had available in this laboratory and from these we were able to determine the unit cell and find the thorium positions. These crystals contain on the order of six water molecules per thorium atom, but the exact composition is in some doubt.

As the crystals were very deliquescent, they were sealed in pyrex capillaries. They were rotated about the [100] axis and rotation and Weissenberg patterns were obtained with Cu Kα radiation (λ = 1.5418 Å). These showed that the crystals were orthorhombic. The following lattice parameters were obtained from powder patterns taken with Cr Kα radiation (λ = 2.2909 Å).

$$\underline{a} = 11.2 \text{ Å}$$

$$\underline{b} = 22.8$$

$$\underline{c} = 10.6$$

These could not be determined to an accuracy greater than 1% because of the complexity of the pattern at high angles.

Determination of Space Group

The following selection rules were observed to hold:

$hk\ell$ only with $h + k = 2n$, $k + \ell = 2n$, and $h + \ell = 2n$,

$h0\ell$ only with $h = 2n$, $\ell = 2n$, and $h + \ell = 4n$,

$0k\ell$ only with $k = 2n$, $\ell = 2n$, and $k + \ell = 4n$,

$hk0$ only with $h = 2n$, and $k = 2n$

which indicates uniquely that the space group is Fdd -- C_{2v}^{19}. A rough determination of the specific gravity gave 2.7 which leads to 7.7 ~8 molecules per unit cell. The density calculated for eight molecules is 2.8. The metals must then occupy the positions

8 (a) (0,0,z; 1/4, 1/4, 1/4 + z,) + F.C.

this set of positions alone has the higher symmetry Fddd -- D_{2h}^{24} which includes a center of symmetry. These crystals exhibit the pyroelectric effect so we know they are not centrosymmetric. In addition this space group would have another selection rule:

hk0 only with h = 2n, k = 2n, and h + k = 4n.

Weak spots were observed which violated this rule. For the special position 8 (a) an additional selection rule:

$hk\ell$ only with $h + k + \ell = 2n \pm 1$ or $4n$

is required, and this rule was also observed to be violated. So some of the atoms must occupy the general positions

16 (b) (x,y,z; $\bar{x},\bar{y}$,z; 1/4 - x, 1/4 + y, 1/4 + z; 1/4 + x, 1/4 - y, 1/4 + z;) + F.C.

No attempt was made to determine the positions of any but the metal atoms as intensity measurements were not considered feasible in view of the large amount of absorption and the size of the crystal.

Table I gives the observed and calculated values for $\sin\theta$ for the first 14 lines, and the observed and calculated intensities calculated for the thorium atoms alone. Beyond this point on the powder pattern the indexing of the lines became quite ambiguous and thus is not reported here.

Table I

hkl	$\sin^2\theta$* obs.	$\sin^2\theta$* calc.	Intensity obs.	Intensity calc.
111	0.0250	0.0246	s	67
040	0.0404	0.0404	m	33
131	0.0449	0.0450	s	65
220	0.0520	0.0522	m	64
022	0.0572	0.0572	m	63
151	0.0855	0.0853	m-	61
202	0.0889	0.0892	w	61
311	0.1090	0.1091	m	59
113	0.1190	0.1189	w	58
331	0.1290	0.1293	m+	58
242		0.1296		115
062	0.1376	0.1380	s	57
133		0.1391		57
171	0.1451	0.1460	w+	56
080	0.1600	0.1616	w	28
400	0.1677	0.1685	m	28
351		0.1697		55

*Cr Kα radiation λ= 2.2909 Å

This work was performed under the auspices of the U. S. Atomic Energy Commission.

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