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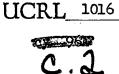
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Publication Date

1950-11-20



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THE CRYSTAL STRUCTURE OF THORIUM NITRATE D. H. Templeton and Carol H. Dauben November 20, 1950



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THE CRYSTAL STRUCTURE OF THORIÚM NITRATE

-3-

D. H. Templeton and Carol H. Dauben Department-of Chemistry and Radiation Laboratory University of California, Berkeley, California

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.

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THE CRYSTAL STRUCTURE OF THORIUM NITRATE

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D. H. Templeton and Carol H. Dauben Department of Chemistry and Radiation Laboratory University of California, Berkeley, California

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 Ka radiation ($\lambda = 1.5418$ Å). These showed that the crystals were orthorhombic. The following lattice parameters were obtained from powder patterns taken with Cr Ka radiation ($\lambda = 2.2909$ Å).

$$\underline{\mathbf{a}} = 11.2 \overset{\text{o}}{\text{A}}$$
$$\underline{\mathbf{b}} = 22.8$$
$$\underline{\mathbf{c}} = 10.6$$

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:

hkl only with h + k = 2n, k + l = 2n, and h + l = 2n, hOl only with h = 2n, l = 2n, and h + l = 4n, Okl only with k = 2n, l = 2n, and k + l = 4n, hkQ 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:

hkO 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:

hkl only with h + k + l = 2n - 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) $(x,y,z; \overline{x},\overline{y},z; 1/4 - x, 1/4 + y, 1/4 + z; 1/4 + x, 1/4 - y, 1/4 + z;) + F.C.$ 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.

hkl	sin	sin ² 0 [*]		Intensity	
	obs.	calc.	obs.	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	
331 242	0.1290	0.1293 0.1296	m+	58 115	
062 133	0.1376	0.1380 0.1391	S	57 57	
171	0.1451	0.1460	W+	56	
080	0.1600	0.1616	W	28	
400 351	0.1677	0.1685 0.1697	m	28 55	

Table I

*Cr Ka radiation λ = 2.2909 Å

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

