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The Crystal Structure of Double Nitrate Octahydrates of Thorium and Bivalent Metals

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X-ray crystal structure analysis of magnesium thorium nitrate hydrate, previously given the formula $MgTh(NO_3)_6 . 8H_2O$, showed that the compound (in the crystal state) is hexa-aquomagnesium hexanitratothorate dihydrate, $Mg(H_2O)_6 . Th(NO_3)_6 . 2H_2O$. It is monoclinic holohedral with the space group $P2_1/c$ (C^5_{2h}). The unit cell, with $a=9\cdot08$, $b=8\cdot75$, $c=13\cdot61$ Å and $\beta=97°$, contains two formula units. The coordinates of all atoms (except hydrogen) were obtained by means of Patterson projections and Fourier and difference Fourier syntheses along [010] and [100].

The crystal structure contains two types of polyhedra around thorium and magnesium atoms (both at the centres of symmetry).

Each thorium atom is surrounded by twelve oxygen atoms which belong to six nitrate ions, the average Th–O distance being 2·63 Å. These oxygen atoms are at the corners of an irregular icosahedron. Each magnesium atom is octahedrally surrounded by six water molecules; the average Mg–O distance is 2·12 Å. The connection between the polyhedra themselves as well as the polyhedra and the remaining (one quarter) "isolated" water molecules is realized through the weak hydrogen bonds.

A series of compounds of general formula $M^{II}Th(NO_3)_6 . 8H_2O$ (M^{II} = Zn, Co, Ni, Mn) is isomorphously related to the described magnesium thorium nitrate hydrate.

Introduction

X-ray crystal structure analysis of double nitrate octahydrates of thorium and bivalent metals forms a part of our wider program of crystallochemical investigations of nitrates and phosphates of tervalent uranium, thorium and cerium with uni- and bivalent metals. The present paper was presented at the VIth International Congress of Crystallography, Rome, Sept. 1963 (Šćavničar & Prodić, 1963).

Preparation, morphology and optical properties of double nitrate octahydrates of thorium and bivalent metals of common formula $M^{II}Th(NO_3)_6 . 8H_2O$ (with M^{II} = Mg, Zn, Co, and Ni) have been known since 1901 (Meyer & Jacoby, 1901; Sachs, 1901; Geipel, 1902). According to our experience the best crystals can be obtained from an equimolar solution of thorium and M^{II} nitrate in dilute (1:1) nitric acid; evaporation of the solution is carried out in a desiccator over sulphuric acid and solid potassium hydroxide and must be slowed down (by removing potassium hydroxide) when the crystallization starts. All these compounds are very deliquescent and unstable so that we had much difficulty in preparing specimens suitable for absorption correction as well as in collecting the necessary X-ray data for structure analysis.

Table 1 contains the parameters of monoclinic (holohedral) unit cells, as determined from oscillation and Weissenberg photographs with Ni-filtered Cu *K* radiation, as well as the values of observed densities (measured by the hydrostatic method in decalin) compared with those calculated for two formula units per unit cell.

The estimated errors are: ±0·007 Å for the lengths of the unit-cell edges, and ±0·3° for β.

All five compounds crystallize in the same space group which is, according to the observed absences of reflexions, $P2_1c$ (C^5_{2h}).

The same symmetry and nearly equal lattice parameters confirm the strict isomorphous relations between the members of the group; this is in accordance with their optical properties (birefringence, orientation of indicatrix, angle of optic axes) and powder diagrams.

Structure determination

Among the five isomorphous substances the crystals of $MgTh(NO_3)_6 . 8H_2O$, as the best developed and most stable, were chosen for further investigation. With the use of an integrating Weissenberg goniometer, normal beam photographs of the *h*0*l* and 0*kl* reflexions were taken from cylindrical specimens (sealed in a

Table 1. *Parameters of unit cells and densities*

	a	b	c	β	ϱ_o	ϱ_c
$MgTh(NO_3)_6 . 8H_2O$	9·08 Å	8·75 Å	13·61 Å	97°	2·41 g.cm^{-3}	2·39 g.cm^{-3}
$MnTh(NO_3)_6 . 8H_2O$	9·08	8·75	13·61	97	2·50	2·48
$CoTh(NO_3)_6 . 8H_2O$	9·08	8·78	13·62	97	2·49	2·49
$NiTh(NO_3)_6 . 8H_2O$	9·08	8·76	13·63	97	2·52	2·49
$ZnTh(NO_3)_6 . 8H_2O$	9·08	8·75	13·63	97	2·54	2·51

capillary tube after quick grinding); the multiple-film technique was applied. Relative intensities of reflexions were deduced from the optical density of each spot measured by means of a microdensitometer. Corrections for polarization and Lorentz factors were made in the usual way. Because of a fairly strong absorption ($\mu=249{\cdot}8$ cm^{-1}) an absorption correction was indispensable and it was carried out with the use of the absorption factors for cylindrical specimens ($\mu \cdot r$ was reduced by grinding to 3·4). The approximate scale factor and the mean isotropic temperature factor were determined by means of the Wilson (1942) statistics.

Patterson $P(xz)$ and $P(yz)$ projections were calculated from the corrected intensity data. It followed from these projections that among four possible twofold positions at centres of symmetry in the $P2_1/c$ space group the positions (*a*) 0, 0, 0; 0, $\frac{1}{2}$, $\frac{1}{2}$ were occupied by thorium atoms, and the positions (*d*) $\frac{1}{2}$, 0, $\frac{1}{2}$; $\frac{1}{2}$, $\frac{1}{2}$, 0 by magnesium atoms. At this stage of the investigation very useful information on the atomic positions of oxygen and nitrogen (general in character) was obtained from Th–O and Th–N maxima in vector maps. The complete structure was successfully solved by means of (010) and (100) electron density projections and difference Fourier syntheses.

No more data were obtained from the electron density projection map along [010] (Fig. 1) by reason of the plus sign of all 155 independent *h*0*l* terms obtained from the Weissenberg photograph. Instead of 60 expected oxygen and nitrogen maxima (the number of these atoms in the unit cell) there were only 48, better or poorer resolved. The seats of superpositions of atoms were easily found from the differences in the heights of maxima. The difference Fourier synthesis, made after rescaling F_o, effected a slight correction of oxygen and nitrogen *x* and *z* coordinates obtained previously from the electron density projection.

About one third of all (152) 0*kl* reflexions, included in the calculation of the electron density projection along [100], had zero intensity (all of them of the type $k+l=2n+1$). The contribution of thorium to the intensity of 0*kl* reflexions with $k+l=2n$ prevailed over the contribution of all the remaining atoms and dictated the plus sign. The first set of signs of 20 observed 0*kl* reflextions with $k+l=2n+1$, for which the structure factors of Th and Mg are zero, was calculated with preliminary *y* coordinates of oxygen and nitrogen atoms deduced from the Patterson projection and from the consideration of all possible atomic arrangements in the available space; the *z* coordinates were known from the (010) projection. After a correction of a few of these signs, on the basis of the first (100) Fourier syntheses, the second electron density projection and then the difference Fourier synthesis, with $(F_o-F_{c(\mathrm{Th+Mg})})$ as coefficients, were calculated. The final values of the coordinates of the atomic positions (except for hydrogen) are given in Table 2.

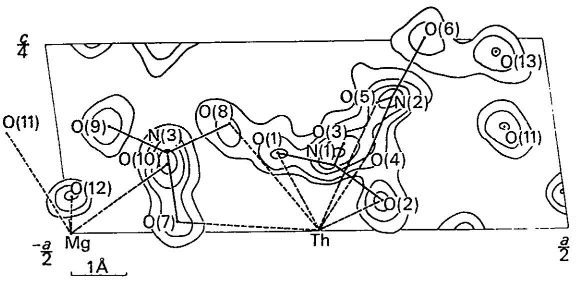

Fig. 1. Contour map of electron density projection along [010] calculated with $(F_o-F_{c(\mathrm{Th+Mg})})$ as coefficients.

Table 2. *Atomic coordinates*

	x	*y*	*z*
Th	0	0	0
Mg	$\frac{1}{2}$	0	$\frac{1}{2}$
O(1)	0·937	0·750	0·104
O(2)	0·133	0·713	0·038
O(3)	0·050	0·543	0·128
O(4)	0·120	0·225	0·112
O(5)	0·150	0·000	0·167
O(6)	0·263	0·184	0·242
O(7)	0·718	0·012	0·012
O(8)	0·850	0·083	0·139
O(9)	0·611	0·050	0·141
O(10) (H_2O)	0·710	0·487	0·087
O(11) (H_2O)	0·395	0·450	0·124
O(12) (H_2O)	0·506	0·740	0·039
O(13) (H_2O)	0·401	0·780	0·223
N(1)	0·040	0·667	0·088
N(2)	0·177	0·135	0·174
N(3)	0·726	0·053	0·098

The observed and the calculated structure factors, included in Table 3, are in good agreement.

The values of the calculated structure factors, F_c, (with omission of hydrogen) were obtained by using the atomic coordinates from Table 2, the atomic scattering factors for neutral atoms from *International Tables for X-ray Crystallography* (1962) with dispersion correction for atomic scattering factor of thorium (*International Tables*, 1962) and individual isotropic temperature factors with $B=1{\cdot}6$ Å^2 for thorium, 2·3 Å^2 for magnesium, and 3·2 Å^2 for oxygen and nitrogen.

From the data of Table 3 the following reliability indices resulted:

$R=0{\cdot}081$ for [010] zone reflexions;

$R=0{\cdot}099$ for [100] zone with all observed (*i.e.* non zero) reflexions included, and $R=0{\cdot}124$ for all 152 possible 0*kl* reflexions.

The difference between $R(0kl)$ calculated from all reflexions and $R(0kl)$ calculated without zero-intensity reflexions is small (2·5%); the introduction of oxygen and nitrogen atoms in F_c (besides thorium and magnesium) lowered *R* values by about 10%. All this speaks in favour of the correctness of the structure, within the limits of the work done with two-dimensional intensity data in the presence of the heavy atom; obtaining three-dimensional intensity data from crystals of such poor stability seemed to us too time consuming to be worth while.

Table 3. *Observed and calculated structure factors*

hkl	F_o	$1/2F_o$
1 0 0	90	99
2 0 0	78	80
3 0 0	58	58
4 0 0	61	56
5 0 0	44	32
6 0 0	51	50
7 0 0	58	57
8 0 0	47	51
9 0 0	14	10
10 0 0	33	31
11 0 0	18	18
0 2 0	105	100
0 4 0	112	131
0 6 0	51	55
0 8 0	40	43
0 10 0	27	26
0 0 2	97	109
0 0 4	45	32
0 0 6	61	63
0 0 8	90	90
0 0 10	53	53
0 0 12	43	41
0 0 14	29	30
0 0 16	23	25
1 0 2	76	75
1 0 $\bar{2}$	87	80
2 0 2	74	64
2 0 $\bar{2}$	117	133
3 0 2	36	32
3 0 $\bar{2}$	92	98
4 0 2	89	97
4 0 $\bar{2}$	69	76
5 0 2	35	33
5 0 $\bar{2}$	21	16

hkl	F_o	$1/2F_o$
6 0 2	52	52
6 0 $\bar{2}$	67	72
7 0 2	40	42
7 0 $\bar{2}$	46	54
8 0 2	43	40
8 0 $\bar{2}$	46	45
9 0 2	25	25
9 0 $\bar{2}$	35	35
10 0 2	24	28
10 0 $\bar{2}$	38	39
11 0 2	19	20
11 0 $\bar{2}$	27	23
1 0 4	58	53
1 0 $\bar{4}$	20	21
2 0 4	51	52
2 0 $\bar{4}$	75	71
3 0 4	42	36
3 0 $\bar{4}$	73	71
4 0 4	82	87
4 0 $\bar{4}$	65	96
5 0 4	45	44
5 0 $\bar{4}$	34	34
6 0 4	45	47
6 0 $\bar{4}$	59	59
7 0 4	40	39
7 0 $\bar{4}$	41	37
8 0 4	46	48
8 0 $\bar{4}$	44	44
9 0 4	29	28
9 0 $\bar{4}$	45	41
10 0 4	24	25
10 0 $\bar{4}$	35	41
11 0 $\bar{4}$	24	30
1 0 6	48	40
1 0 $\bar{6}$	67	70

hkl	F_o	$1/2F_c$
2 0 6	57	62
2 0 $\bar{6}$	66	70
3 0 6	27	28
3 0 $\bar{6}$	32	31
4 0 6	55	50
4 0 $\bar{6}$	36	36
5 0 6	58	55
5 0 $\bar{6}$	48	47
6 0 6	55	59
6 0 $\bar{6}$	62	66
7 0 6	34	37
7 0 $\bar{6}$	39	36
8 0 6	31	30
8 0 $\bar{6}$	45	46
9 0 6	27	25
9 0 $\bar{6}$	32	30
10 0 6	21	25
10 0 $\bar{6}$	33	28
11 0 $\bar{6}$	22	19
1 0 8	49	47
1 0 $\bar{8}$	52	55
2 0 8	51	43
2 0 $\bar{8}$	71	76
3 0 8	62	62
3 0 $\bar{8}$	47	51
4 0 8	34	30
4 0 $\bar{8}$	48	54
5 0 8	40	39
5 0 $\bar{8}$	40	40
6 0 8	26	34
6 0 $\bar{8}$	24	25
7 0 8	31	27
7 0 8	42	42
8 0 8	27	32
8 0 $\bar{8}$	37	40

hkl	F_o	$1/2F_o$
9 0 8	19	19
9 0 $\bar{8}$	21	21
10 0 $\bar{8}$	26	26
1 0 10	55	45
1 0 $\overline{10}$	58	51
2 0 10	60	53
2 0 $\overline{10}$	43	41
3 0 10	41	42
3 0 $\overline{10}$	59	61
4 0 10	44	43
4 0 $\overline{10}$	52	58
5 0 10	32	24
5 0 $\overline{10}$	34	36
6 0 10	33	29
6 0 $\overline{10}$	29	34
7 0 10	31	31
7 0 $\overline{10}$	26	24
8 0 10	22	21
8 0 $\overline{10}$	27	28
9 0 $\overline{10}$	22	24
10 0 $\overline{10}$	27	29
1 0 12	40	40
1 0 $\overline{12}$	47	37
2 0 12	22	23
2 0 $\overline{12}$	41	41
3 0 12	34	31
3 0 $\overline{12}$	44	48
4 0 12	40	42
4 0 $\overline{12}$	41	42
5 0 12	31	32
5 0 $\overline{12}$	18	19
6 0 12	29	28
6 0 $\overline{12}$	36	36
7 0 12	18	24
7 0 $\overline{12}$	31	32

hkl	F_o	$1/2F_c$
8 0 $\overline{12}$	26	23
9 0 $\overline{12}$	21	23
1 0 14	23	27
1 0 $\overline{14}$	24	23
2 0 14	29	30
2 0 $\overline{14}$	40	38
3 0 14	34	30
3 0 $\overline{14}$	36	36
4 0 14	30	30
4 0 $\overline{14}$	26	26
5 0 14	25	28
5 0 $\overline{14}$	26	30
6 0 $\overline{14}$	27	30
7 0 $\overline{14}$	24	25
1 0 16	25	30
1 0 $\overline{16}$	14	17
2 0 16	22	25
2 0 $\overline{16}$	22	26
3 0 $\overline{16}$	22	25
4 0 $\overline{16}$	28	30
5 0 $\overline{16}$	25	29
0 1 1	92	88
0 1 2	0	2
0 1 3	51	52
0 1 4	31	30
0 1 5	86	95
0 1 6	34	29
0 1 7	69	73
0 1 8	0	1
0 1 9	43	41
0 1 10	0	4
0 1 11	38	38
0 1 12	0	2
0 1 13	31	37
0 1 14	0	1
0 1 15	20	23

hkl	F_o	$1/2F_c$
0 1 16	0	−1
0 1 17	16	21
0 2 1	39	−42
0 2 2	79	90
0 2 3	17	−22
0 2 4	37	39
0 2 5	11	7
0 2 6	86	99
0 2 7	0	3
0 2 8	90	70
0 2 9	6	−7
0 2 10	60	52
0 2 11	0	3
0 2 12	47	47
0 2 13	0	−3
0 2 14	32	38
0 2 15	0	0
0 2 16	26	30
0 3 1	66	78
0 3 2	47	−35
0 3 3	71	83
0 3 4	12	−8
0 3 5	61	68
0 3 6	0	−5
0 3 7	57	59
0 3 8	0	0
0 3 9	25	34
0 3 10	6	−7
0 3 11	38	31
0 3 12	0	1
0 3 13	31	31
0 3 14	0	−2
0 3 15	22	23
0 3 16	0	0
0 4 1	0	−2
0 4 2	84	83

Table 3 (*cont.*)

hkl	F_o	$1/2F_c$
0 4 3	6	2
0 4 4	59	63
0 4 5	20	21
0 4 6	49	56
0 4 7	0	2
0 4 8	63	61
0 4 9	0	−3
0 4 10	47	49
0 4 11	0	0
0 4 12	35	34
0 4 13	5	6
0 4 14	27	28
0 4 15	0	−4
0 4 16	19	22
0 5 1	35	45
0 5 2	7	−10
0 5 3	39	47
0 5 4	0	−4
0 5 5	48	60
0 5 6	19	17
0 5 7	45	44
0 5 8	13	9
0 5 9	47	43
0 5 10	0	1
0 5 11	32	32
0 5 12	0	0
0 5 13	26	29
0 5 14	0	−1
0 5 15	15	20
0 6 1	0	−4
0 6 2	47	53
0 6 3	14	−12
0 6 4	61	63
0 6 5	0	−2
0 6 6	46	49

hkl	F_o	$1/2F_c$
0 6 7	2	4
0 6 8	34	37
0 6 9	9	−8
0 6 10	38	38
0 6 11	0	−2
0 6 12	39	41
0 6 13	0	0
0 6 14	25	29
0 7 1	45	41
0 7 2	0	−5
0 7 3	44	45
0 7 4	0	−4
0 7 5	42	48
0 7 6	0	−2
0 7 7	36	38
0 7 8	0	4
0 7 9	22	21
0 7 10	0	−3
0 7 11	26	26
0 7 12	0	−1
0 7 13	19	19
0 8 1	0	−2
0 8 2	45	46
0 8 3	5	6
0 8 4	44	46
0 8 5	0	0
0 8 6	44	41
0 8 7	0	3
0 8 8	26	26
0 8 9	0	2
0 8 10	31	32
0 8 11	0	1
0 8 12	24	28
0 9 1	35	31

hkl	F_o	$1/2F_c$
0 9 2	0	1
0 9 3	23	23
0 9 4	0	1
0 9 5	24	28
0 9 6	0	−2
0 9 7	26	27
0 9 8	0	0
0 9 9	28	26
0 9 10	0	3
0 10 1	0	2
0 10 2	27	26
0 10 3	0	−2
0 10 4	35	35
0 10 5	0	1
0 10 6	28	29
0 10 7	0	−3
0 11 1	21	22
0 11 2	0	−1
0 11 3	19	22

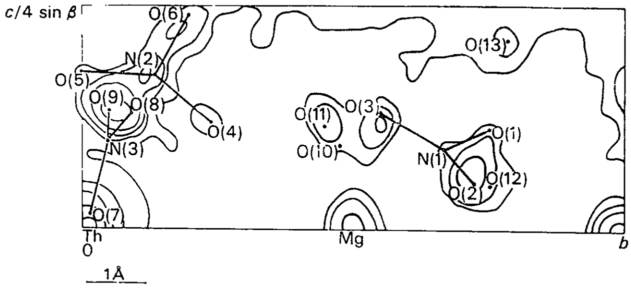

Fig. 2. Contour map of electron density projection along [100], with an interval of contour lines for thorium ten times that for light atoms.

Description and discussion of the structure

Taking into account only the relations between the coordination numbers of cations (derived from the ratios of ionic radii) and the composition of the compound, one could be misled to accept a simple formula $[Th(H_2O)_8]$. $[Mg(NO_3)_6]$, for the ratio of number of water molecules to the number of thorium atoms is equal the coordination number of Th^{4+}, and the number of nitrate ions per magnesium atom is equal to the coordination number of Mg^{2+}.

The results of the reported investigation of crystal structure have shown that the proper structural formula is $[Mg(H_2O)_6].[Th(NO_3)_6].2H_2O$, which reflects the real state of coordination. In the structure of this hydrated magnesium thorium double nitrate each magnesium atom (in the (*d*) position) is surrounded by six water molecules disposed at the corners of a nearly regular octahedron (as seen from the values of lengths of octahedral edges, Table 4). The average Mg–OH_2 distance of 2·12 Å slightly exceeds the sum of ionic radii (taking the values of radii from Pauling (1960), *i.e.* 0·65 for Mg^{2+} and 1·40 Å for O^{2-}). Water molecules around the magnesium ion do not enter into the sphere of stronger action of the thorium ion.

Table 4. *Bond lengths and interatomic distances*

(Estimated to be accurate within 0·05 Å)

(*a*) Within the icosahedron around thorium

Th–O(1)	2·72 Å		O(1) ··· O(7)	3·19 Å
Th–O(2)	2·80		O(1) ··· O(8)	3·05
Th–O(4)	2·62		O(2) ··· O(4′)	2·91
Th–O(5)	2·50		O(2) ··· O(5)	3·06
Th–O(7)	2·58		O(2) ··· O(7′)	2·78
Th–O(8)	2·57		O(2) ··· O(8′)	3·02
O(1) ··· O(2)	2·12	edges of three NO_3 triangles	O(4) ··· O(7′)	3·15
O(4) ··· O(5)	2·11		O(4) ··· O(8)	2·81
O(7) ··· O(8)	2·08		O(5) ··· O(7′)	2·84
O(1) ··· O(4′)	2·93		O(5) ··· O(8)	2·79
O(1) ··· O(5)	2·98			

(*b*) Within the octahedron around magnesium

Mg–O(10)	2·12 Å	O(10) ··· O(12)	2·91 Å
Mg–O(11)	2·09	O(10) ··· O(12′)	3·14
Mg–O(12)	2·16	O(11) ··· O(12)	3·00
O(10) ··· O(11)	2·98	O(11) ··· O(12′)	3·00
O(10) ··· O(11′)	2·96		

(*c*) Between polyhedra (less than 3·1 Å)

O(3) ··· O(4)	2·98 Å	O(6″) ··· O(10)	2·88 Å
O(1) ··· O(6″)	3·00	O(7) ··· O(12′)	2·99
O(1) ··· O(10)	3·08	O(9) ··· O(12)	3·08
O(2′) ··· O(10)	2·92		

(*d*) Between "isolated" water molecules and neighbouring oxygen atoms.

O(13) ··· O(5)	3·01 Å	O(13″) ··· O(11)	3·00 Å
O(13″) ··· O(9)	2·74	O(13) ··· O(12)	2·98

O′ and O″ stand for the atoms which are related through a center of symmetry (O′) or screw (O″) to the atoms of the same index listed in Table 2.

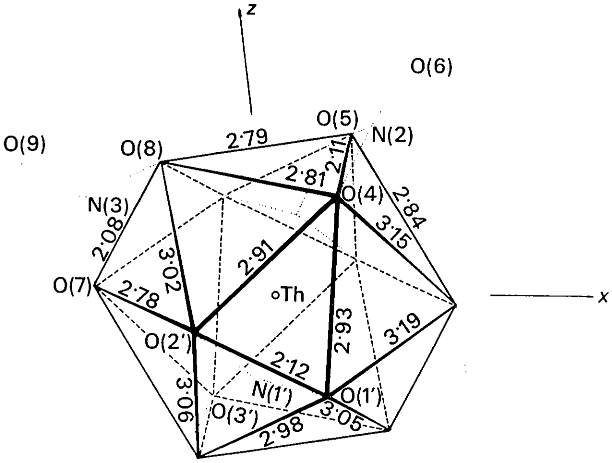

Fig. 3. Icosahedron around the thorium ion, as seen along (010).

Each thorium atom is surrounded by twelve oxygen atoms of nitrate ions. Because of a centrosymmetrical position [position (*a*)] of thorium, the coordination polyhedron around it should have at least a center of symmetry. In fact neighbouring oxygen atoms belong to three pairs of centrosymmetrically related nitrate ions and form a polyhedron, which is composed of twenty triangular faces (Fig. 3). Twelve faces approximate to an isosceles triangle (with sides: $a\sim 2·1$, $b\sim c\sim 2·9$ Å), and eight faces are acute triangles (with sides from 2·8 to 3·2 Å). Such a body with twenty triangular faces and a center of symmetry (as the only element of symmetry) may be called an "irregular icosahedron". The lengths of the Th–O distances (Table 4) are from 0·1 to 0·4 Å greater than the sum of ionic radii (*i.e.* 2·425 Å in the fluorite type structure of ThO_2). The variation of thorium to oxygen distances is appreciable, from 2·50 Å to 2·80 Å, the average distance being 2·63 Å.

According to the data of Table 2, N–O bond distances are equal to 1·22 Å (±0·07 Å) without any remarkable difference in each nitrate ion between the two oxygen atoms bonded to thorium and the third one; an exception is N(3)–O(9) with 1·27 Å.

Twelve as a coordination number of thorium is unexpectedly large; it can be understood and explained by the fact that instead of twelve mutually non-bonded oxygen atoms there are six diatomic groups (from six nitrate ions) having an O ··· O distance of about 2·1 Å (edge of NO_3 triangle), which is considerably less than the sum of atomic radii.

The gathering of the nitrate ions around the thorium and the water molecules around the magnesium could have its reason in the greater ionic potential (charge/radius) of Th^{4+} as compared with the ionic potential of Mg^{2+}.

One quarter of the water molecules do not participate in the formation of the coordination polyhedra around the metal atoms, and can be regarded as isolated water of crystallization.

The icosahedron and the octahedron do not share either edges or corners. Connection between them is effected through a water–oxygen interaction (Fig. 4), which may be interpreted by hydrogen bonds $H_2O(10)-O(6)=2·88$ Å, $H_2O(10)-O(2)=2·92$ Å, $H_2O(12)-O(7)=2·99$ Å. The octahedron fits well into the space left over between the icosahedra and the isolated water molecules. The water of crystallization has four nearest neighbours at the corners of a very flattened tetrahedron: O(9) at 2·74, O(5) at 3·01, $H_2O(11)$ at 3·00 and $H_2O(12)$ at 2·98 Å. In this way it also functions as a connection between the octahedra and the icosahedra.

Quite recently our attention was drawn to the paper of Zalkin, Forrester & Templeton (1963) on the crystal structure of cerium(III) magnesium nitrate hydrate, determined very carefully with three-dimen-

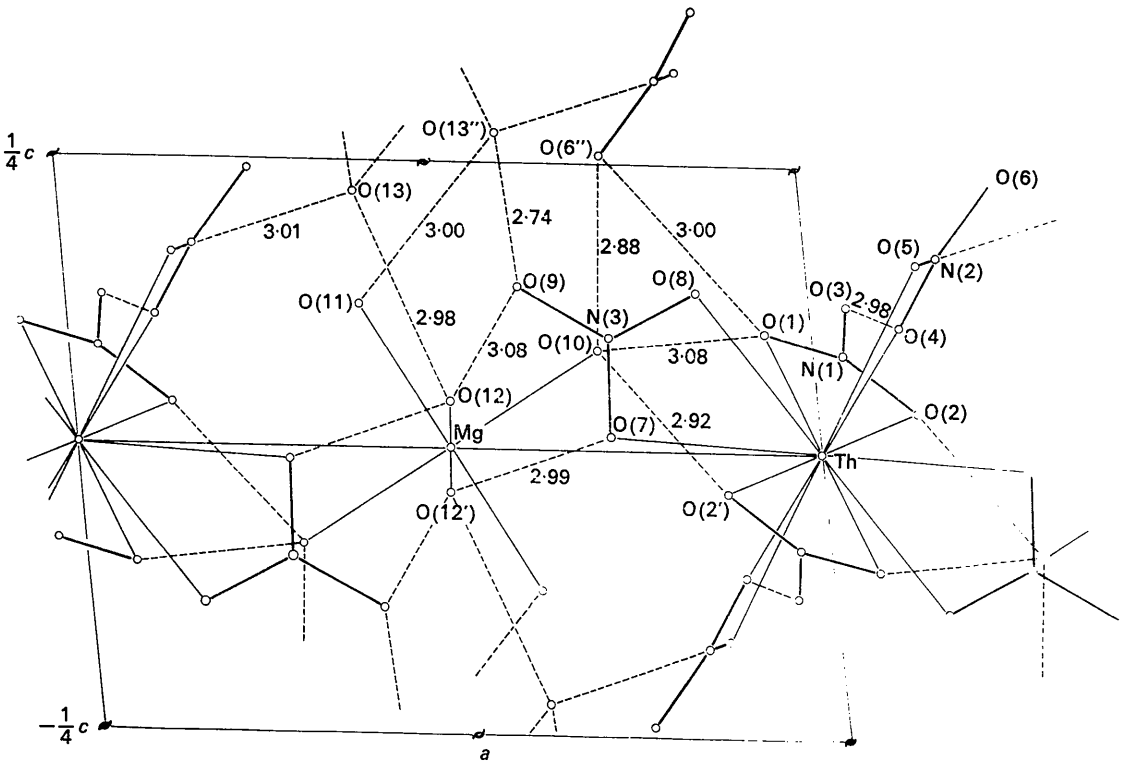

Fig. 4. Schematic representation of the structure in the (010) projection. Nitrate ions are shown by heavy lines; Th–O and Mg–H_2O bonds are traced by thin lines. Dashed lines connect atoms of different polyhedra and isolated water molecules; only distances shorter than 3·1 Å are taken into account.

sional data. Comparison of the trigonal structure of magnesium cerium(III) nitrate hydrate with the monoclinic structure of magnesium thorium(IV) nitrate octahydrate reveals a surprising similarity as to the distribution of nitrate ions and water molecules around the cations, the coordination numbers and types of polyhedra, and the average values of metal to oxygen distances.

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