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Thorium divanadate dihydrate, Th(V₂O₇)(H₂O)₂

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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{Th}-\text{O}) = 0.002$ Å; R factor = 0.014; wR factor = 0.033; data-to-parameter ratio = 32.5.

The title compound, Th(V₂O₇)(H₂O)₂, was synthesized by a hydrothermal reaction. The crystal structure consists of ThO₇(OH)₂ tricapped trigonal prisms that share edges, forming [ThO₅(OH)₂]_n chains along [010]. The edge-sharing ThO₇(OH)₂ polyhedra share one edge and five vertices with the V₂O₇ divanadate anions having a nearly ecliptic conformation parallel to [001]. This results in an open framework with the water molecules located in channels. O—H...O hydrogen bonding between water molecules and framework O atoms is observed. Bond-valence-sum calculations are in good agreement with the chemical formula of the title compound.

Related literature

For thorium compounds with ninefold coordination of the metal, see: Matkovic *et al.* (1968); Boatner (2002); Sullens & Albrecht-Schmitt (2005); Sullens *et al.* (2006); Calestani & Andreotti (1984); Kojić-Prodić *et al.* (1982). For bond-valence sums, see: Brese & O'Keeffe (1991).

Experimental

Crystal data

Th(V₂O₇)(H₂O)₂
 $M_r = 481.95$
Triclinic, $P\bar{1}$
 $a = 7.0432$ (4) Å
 $b = 7.3702$ (4) Å
 $c = 7.7204$ (4) Å

$\alpha = 77.849$ (2)°
 $\beta = 74.831$ (2)°
 $\gamma = 85.934$ (2)°
 $V = 378.08$ (4) Å³
 $Z = 2$
Mo $K\alpha$ radiation

$\mu = 22.06$ mm⁻¹
 $T = 296$ K

0.19 × 0.12 × 0.10 mm

Data collection

Bruker X8 APEXII diffractometer
Absorption correction: multi-scan
(SADABS; Bruker, 2005)
 $T_{\min} = 0.052$, $T_{\max} = 0.110$

15216 measured reflections
3576 independent reflections
3506 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.014$
 $wR(F^2) = 0.033$
 $S = 1.15$
3576 reflections

110 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 1.60$ e Å⁻³
 $\Delta\rho_{\min} = -1.26$ e Å⁻³

Table 1
Hydrogen-bond geometry (Å, °).

| D—H...A | D—H | H...A | D...A | D—H...A |
|----------------------------|------|-------|-----------|---------|
| O8—H8A...O4 ⁱ | 0.86 | 2.47 | 3.114 (3) | 133 |
| O8—H8B...O5 ⁱⁱ | 0.86 | 1.92 | 2.779 (3) | 175 |
| O9—H9A...O1 ⁱⁱⁱ | 0.86 | 1.77 | 2.594 (3) | 160 |
| O9—H9B...O5 ^{iv} | 0.86 | 1.90 | 2.741 (3) | 166 |

Symmetry codes: (i) $x, y, z + 1$; (ii) $x - 1, y, z + 1$; (iii) $-x + 1, -y, -z + 1$; (iv) $x - 1, y, z$.

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2454).

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Thorium divanadate dihydrate, $\text{Th}(\text{V}_2\text{O}_7)(\text{H}_2\text{O})_2$ **Said Yagoubi, Lahcen El Ammari, Abderrazzak Assani and Mohamed Saadi****S1. Comment**

As reported in the literature, a few structures with ninefold coordination of thorium have been observed. In the case of orthophosphates and orthoarsenates, only two structure-types exist: the monoclinic $\text{KTh}_2(\text{PO}_4)_3$ (space group $C2/c$) (Matkovic *et al.* 1968) and the monazite CePO_4 (space group $P21/n$) structures (Boatner, 2002). The $\text{KTh}_2(\text{PO}_4)_3$ structure is built from corrugated sheets parallel to (100) face of thorium polyhedra ThO_9 sharing edges. Phosphate tetrahedral share vertices and edges with the thorium polyhedra to define a framework with channels occupied by K atoms. For the monazite compound, the structure shows a parallel chains to [010] direction, formed by CeO_9 polyhedra that share edges. These infinite chains are connected together by edge-sharing with phosphate tetrahedra to form sheets parallel to the (100) face. The stacking of these layers along [100] direction by further edge-sharing of the CeO_9 polyhedra forms a three-dimensional framework. These two structure-types ($\text{KTh}_2(\text{PO}_4)_3$ and CePO_4) are amongst the most important as they show the widest range of chemical composition. Dimers of edges-shared ThO_9 are found in $\text{Na}_6[\text{Th}(\text{PO}_4)(\text{P}_2\text{O}_7)]_2$ (space group $P-1$) (Kojić-Prodić, *et al.*, 1982). These dimers are connected together by sharing edges with phosphate tetrahedral into double chains along [100] direction. Pyrophosphate groups share vertices with the double chains and define a framework with channels occupied by Na atoms. Five other Th(IV) compounds with ninefold coordination and heavy oxoanions were cited in the literature: four structures containing mixed geometry anions were published by Sullens & Albrecht-Schmitt (2005); Sullens *et al.* (2006), $\text{Th}(\text{VO}_2)_2(\text{TeO}_6)(\text{H}_2\text{O})_2$, $\text{Th}(\text{SeO}_3)(\text{SeO}_4)$, $\text{Th}(\text{IO}_3)_2(\text{SeO}_4)(\text{H}_2\text{O})_3$, H_2O and $\text{Th}(\text{CrO}_4)(\text{IO}_3)_2$ and one compound with mixed site $\text{Pb}_{0.5}\text{Th}_{0.5}\text{VO}_4$ was published by Calestani & Andreotti (1984). For all these compounds, each ThO_9 (or ThPbO_9) polyhedra is bounded by the oxoanions groups.

In an effort to understand the structural chemistry of vanadate with actinides, we obtained the following compound of formula $\text{Th}(\text{V}_2\text{O}_7)(\text{H}_2\text{O})_2$ under mild hydrothermal conditions. The structure of this compound consists of $\text{ThO}_7(\text{OH}_2)_2$ tricapped trigonal prisms that share edges to form chains $[\text{ThO}_5(\text{OH}_2)_2]_\infty$ along the [010] direction. The edge-sharing $\text{ThO}_7(\text{OH}_2)_2$ polyhedra share one edge and five vertices with the V_2O_7 divanadate anions parallel to [001] direction. That builds an open framework with water molecules pointing towards the tunnels. The bond-valence sums were calculated using the coordination-independent parameters given by Brese and O'Keeffe (1991). The obtained value are as follows: Th1, 4.06; V1, 5.10 and V2, 5.18. The two oxygen atoms (O8 and O9) are concluded to be water molecules on the basis of their high isotropic displacement parameters, their bond valence sums of 0.34 (O8) and 0.47(O9), charge balance requirements. That gives the structural formula $\text{Th}(\text{V}_2\text{O}_7)(\text{H}_2\text{O})_2$ for the studied compound.

S2. Experimental

Crystals of $\text{Th}(\text{V}_2\text{O}_7)(\text{H}_2\text{O})_2$, were hydrothermally synthesized in a 25 ml Teflon-lined steel autoclave from two mixtures: $\text{Th}(\text{NO}_3)_4(\text{H}_2\text{O})_4$, NH_4VO_3 and V_2O_5 in the equimolar ratio or $\text{Th}(\text{NO}_3)_4(\text{H}_2\text{O})_4$ and V_2O_5 in the molar ratio 4:3. Ten ml of distilled water was added in each mixture with $\text{pH} = 4.5$. The autoclaves were heated 7 days at 403 K then 2 days at 483 K followed by slow cooling to room temperature. The resulting product was recovered by filtration, washed with

deionized water and finally air dried. The reaction product consists of orange powder and some yellow-colored crystals corresponding to the title compound which they can be isolated using ultrasonic.

S3. Refinement

The O-bound H atoms were initially located in a difference map and refined with O—H distance restraints of 0.86 (1). In the last cycle they were refined in the riding model approximation with $U_{\text{iso}}(\text{H})$ set to $1.2U_{\text{eq}}(\text{O})$. The highest and deepest hole residual peak in the final difference Fourier map are located at 0.67 Å and 0.88 Å, from Th1. The non significant distances and angles are removed from the cif file.

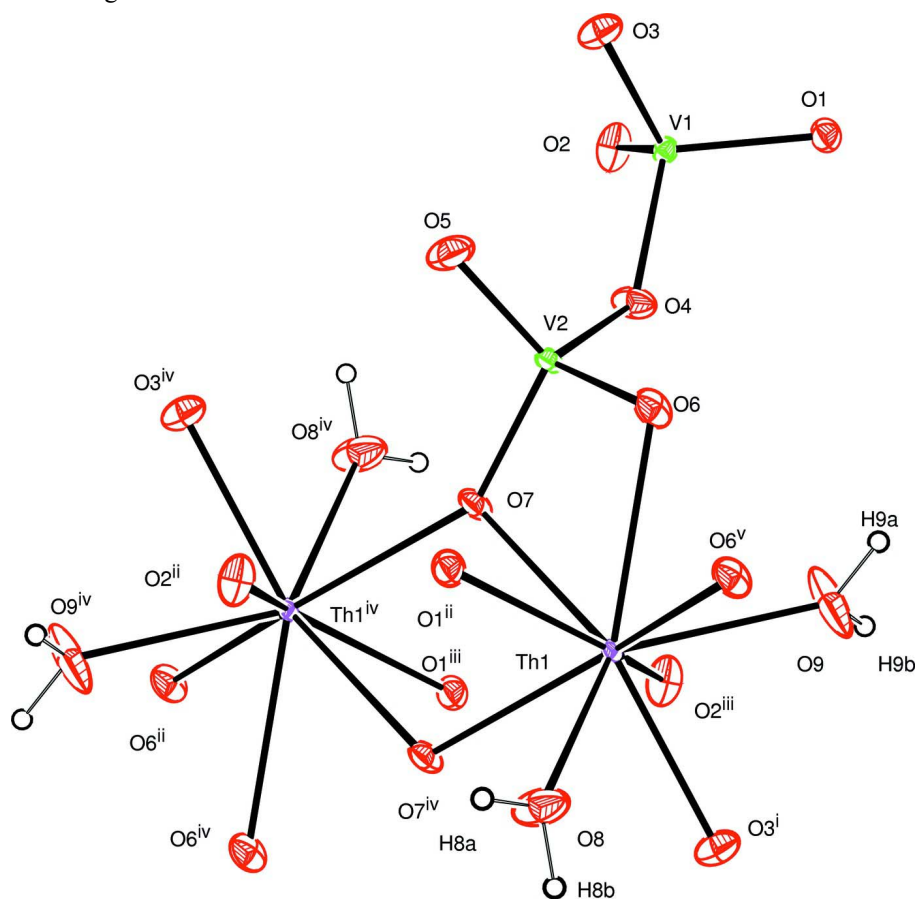


Figure 1

Partial plot of $\text{Th}(\text{V}_2\text{O}_7)(\text{H}_2\text{O})_2$ crystal structure. Displacement ellipsoids are drawn at the 50% probability level.

Symmetry codes: (i) $x - 1, y, z + 1$; (ii) $x, y, z + 1$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $-x + 1, -y + 1, -z + 2$; (v) $-x + 1, -y, -z + 2$; (vi) $-x + 1, -y, -z + 1$; (vii) $x - 1, y, z$.

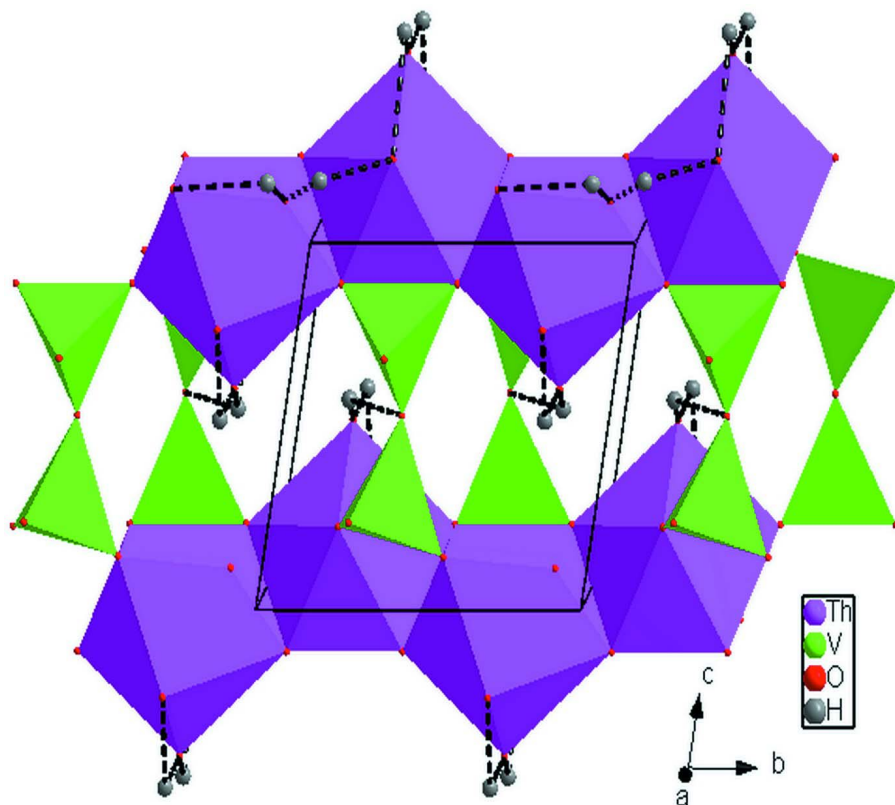


Figure 2

A three-dimensional polyhedral view of the crystal structure of the $\text{Th}(\text{V}_2\text{O}_7)(\text{H}_2\text{O})_2$ showing polyhedra linkage.

Thorium divanadate dihydrate

Crystal data

$\text{Th}(\text{V}_2\text{O}_7)(\text{H}_2\text{O})_2$
 $M_r = 481.95$
 Triclinic, $P\bar{1}$
 Hall symbol: $-P\ 1$
 $a = 7.0432(4)\ \text{\AA}$
 $b = 7.3702(4)\ \text{\AA}$
 $c = 7.7204(4)\ \text{\AA}$
 $\alpha = 77.849(2)^\circ$
 $\beta = 74.831(2)^\circ$
 $\gamma = 85.934(2)^\circ$
 $V = 378.08(4)\ \text{\AA}^3$

$Z = 2$
 $F(000) = 424$
 $D_x = 4.233\ \text{Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$
 Cell parameters from 3576 reflections
 $\theta = 2.8\text{--}36.0^\circ$
 $\mu = 22.06\ \text{mm}^{-1}$
 $T = 296\ \text{K}$
 Prism, yellow
 $0.19 \times 0.12 \times 0.10\ \text{mm}$

Data collection

Bruker X8 APEXII
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2005)
 $T_{\min} = 0.052$, $T_{\max} = 0.110$

15216 measured reflections
 3576 independent reflections
 3506 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$
 $\theta_{\max} = 36.0^\circ$, $\theta_{\min} = 2.8^\circ$
 $h = -11 \rightarrow 11$
 $k = -12 \rightarrow 12$
 $l = -12 \rightarrow 12$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.014$
 $wR(F^2) = 0.033$
 $S = 1.15$
 3576 reflections
 110 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: difference Fourier map
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0019P)^2 + 0.3878P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.003$
 $\Delta\rho_{\max} = 1.60 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.26 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0083 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against all reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on all data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| Th1 | 0.358260 (9) | 0.244262 (9) | 1.084559 (8) | 0.00611 (3) |
| V1 | 0.79469 (5) | 0.33646 (5) | 0.25516 (4) | 0.00702 (6) |
| V2 | 0.72488 (5) | 0.29521 (5) | 0.70555 (4) | 0.00705 (6) |
| O7 | 0.6164 (2) | 0.4536 (2) | 0.8411 (2) | 0.0112 (3) |
| O1 | 0.6561 (2) | 0.2001 (2) | 0.1850 (2) | 0.0122 (3) |
| O6 | 0.6084 (3) | 0.0958 (2) | 0.8397 (2) | 0.0137 (3) |
| O3 | 1.0237 (2) | 0.2469 (2) | 0.2411 (2) | 0.0153 (3) |
| O2 | 0.7983 (3) | 0.5430 (2) | 0.1207 (2) | 0.0162 (3) |
| O4 | 0.6682 (3) | 0.3462 (2) | 0.4897 (2) | 0.0151 (3) |
| O5 | 0.9622 (3) | 0.2782 (3) | 0.6782 (2) | 0.0191 (3) |
| O8 | 0.2995 (3) | 0.1801 (3) | 1.4332 (2) | 0.0250 (4) |
| H8A | 0.3836 | 0.1644 | 1.4984 | 0.030* |
| H8B | 0.1908 | 0.2063 | 1.5061 | 0.030* |
| O9 | 0.1870 (4) | 0.1056 (3) | 0.9082 (4) | 0.0366 (6) |
| H9A | 0.2211 | 0.0097 | 0.8594 | 0.044* |
| H9B | 0.1036 | 0.1642 | 0.8519 | 0.044* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|---------------|---------------|
| Th1 | 0.00668 (4) | 0.00456 (3) | 0.00738 (3) | 0.00008 (2) | -0.00182 (2) | -0.00181 (2) |
| V1 | 0.00677 (13) | 0.00767 (13) | 0.00671 (12) | -0.00029 (10) | -0.00215 (10) | -0.00106 (10) |
| V2 | 0.00842 (13) | 0.00610 (13) | 0.00644 (12) | 0.00028 (10) | -0.00092 (10) | -0.00219 (10) |

| | | | | | | |
|----|-------------|-------------|-------------|-------------|--------------|--------------|
| O7 | 0.0146 (7) | 0.0082 (6) | 0.0112 (6) | 0.0006 (5) | -0.0021 (5) | -0.0050 (5) |
| O1 | 0.0109 (6) | 0.0117 (7) | 0.0160 (6) | 0.0013 (5) | -0.0050 (5) | -0.0054 (5) |
| O6 | 0.0204 (8) | 0.0070 (6) | 0.0129 (6) | -0.0018 (6) | -0.0026 (6) | -0.0016 (5) |
| O3 | 0.0097 (6) | 0.0200 (8) | 0.0139 (6) | 0.0018 (6) | -0.0020 (5) | -0.0006 (6) |
| O2 | 0.0186 (8) | 0.0122 (7) | 0.0176 (7) | -0.0045 (6) | -0.0092 (6) | 0.0049 (6) |
| O4 | 0.0159 (7) | 0.0211 (8) | 0.0084 (6) | 0.0043 (6) | -0.0033 (5) | -0.0046 (5) |
| O5 | 0.0100 (7) | 0.0303 (10) | 0.0163 (7) | 0.0025 (7) | -0.0016 (6) | -0.0063 (7) |
| O8 | 0.0151 (8) | 0.0467 (13) | 0.0123 (7) | 0.0038 (8) | -0.0024 (6) | -0.0066 (7) |
| O9 | 0.0460 (13) | 0.0252 (10) | 0.0645 (15) | 0.0236 (10) | -0.0464 (13) | -0.0327 (11) |

Geometric parameters (Å, °)

| | | | |
|---|-------------|---------------------------|-------------|
| Th1—O3 ⁱ | 2.3508 (16) | V1—O1 | 1.7037 (16) |
| Th1—O1 ⁱⁱ | 2.3988 (15) | V1—O4 | 1.8109 (16) |
| Th1—O2 ⁱⁱⁱ | 2.4104 (15) | V2—O5 | 1.6285 (17) |
| Th1—O7 ^{iv} | 2.4430 (16) | V2—O6 | 1.7296 (16) |
| Th1—O9 | 2.4440 (19) | V2—O7 | 1.7351 (16) |
| Th1—O6 ^v | 2.4598 (16) | V2—O4 | 1.7722 (15) |
| Th1—O8 | 2.5593 (17) | O8—H8A | 0.8599 |
| Th1—O7 | 2.5706 (16) | O8—H8B | 0.8599 |
| Th1—O6 | 2.5937 (17) | O9—H9A | 0.8600 |
| V1—O2 | 1.6498 (16) | O9—H9B | 0.8600 |
| V1—O3 | 1.6845 (16) | | |
| O3 ⁱ —Th1—O1 ⁱⁱ | 133.04 (5) | O6 ^v —Th1—O7 | 123.52 (5) |
| O3 ⁱ —Th1—O2 ⁱⁱⁱ | 74.96 (6) | O8—Th1—O7 | 128.58 (6) |
| O1 ⁱⁱ —Th1—O2 ⁱⁱⁱ | 141.47 (6) | O3 ⁱ —Th1—O6 | 142.46 (6) |
| O3 ⁱ —Th1—O7 ^{iv} | 87.85 (6) | O1 ⁱⁱ —Th1—O6 | 74.59 (5) |
| O1 ⁱⁱ —Th1—O7 ^{iv} | 79.21 (5) | O2 ⁱⁱⁱ —Th1—O6 | 97.58 (6) |
| O2 ⁱⁱⁱ —Th1—O7 ^{iv} | 75.88 (6) | O7 ^{iv} —Th1—O6 | 126.68 (5) |
| O3 ⁱ —Th1—O9 | 74.46 (8) | O9—Th1—O6 | 69.48 (7) |
| O1 ⁱⁱ —Th1—O9 | 139.27 (6) | O6 ^v —Th1—O6 | 64.61 (6) |
| O2 ⁱⁱⁱ —Th1—O9 | 63.63 (7) | O8—Th1—O6 | 130.52 (6) |
| O7 ^{iv} —Th1—O9 | 138.65 (6) | O7—Th1—O6 | 61.59 (5) |
| O3 ⁱ —Th1—O6 ^v | 93.95 (6) | O2—V1—O3 | 111.26 (9) |
| O1 ⁱⁱ —Th1—O6 ^v | 77.24 (6) | O2—V1—O1 | 106.38 (8) |
| O2 ⁱⁱⁱ —Th1—O6 ^v | 134.16 (6) | O3—V1—O1 | 110.92 (8) |
| O7 ^{iv} —Th1—O6 ^v | 149.25 (5) | O2—V1—O4 | 110.99 (9) |
| O9—Th1—O6 ^v | 70.53 (6) | O3—V1—O4 | 111.03 (8) |
| O3 ⁱ —Th1—O8 | 66.51 (6) | O1—V1—O4 | 106.04 (8) |
| O1 ⁱⁱ —Th1—O8 | 66.54 (6) | O5—V2—O6 | 111.61 (9) |
| O2 ⁱⁱⁱ —Th1—O8 | 131.90 (7) | O5—V2—O7 | 112.45 (9) |
| O7 ^{iv} —Th1—O8 | 75.03 (6) | O6—V2—O7 | 99.47 (8) |
| O9—Th1—O8 | 126.93 (8) | O5—V2—O4 | 110.14 (8) |
| O6 ^v —Th1—O8 | 77.61 (6) | O6—V2—O4 | 110.71 (8) |
| O3 ⁱ —Th1—O7 | 140.50 (5) | O7—V2—O4 | 112.08 (8) |
| O1 ⁱⁱ —Th1—O7 | 73.42 (5) | V2—O4—V1 | 136.90 (10) |
| O2 ⁱⁱⁱ —Th1—O7 | 69.92 (5) | H8A—O8—H8B | 104.5 |

| | | | |
|--------------------------|------------|------------|-------|
| O7 ^{iv} —Th1—O7 | 66.76 (6) | H9A—O9—H9B | 104.5 |
| O9—Th1—O7 | 104.44 (8) | | |

Symmetry codes: (i) $x-1, y, z+1$; (ii) $x, y, z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+1, -y+1, -z+2$; (v) $-x+1, -y, -z+2$.

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O8—H8A \cdots O4 ⁱⁱ | 0.86 | 2.47 | 3.114 (3) | 133 |
| O8—H8B \cdots O5 ⁱ | 0.86 | 1.92 | 2.779 (3) | 175 |
| O9—H9A \cdots O1 ^{vi} | 0.86 | 1.77 | 2.594 (3) | 160 |
| O9—H9B \cdots O5 ^{vii} | 0.86 | 1.90 | 2.741 (3) | 166 |

Symmetry codes: (i) $x-1, y, z+1$; (ii) $x, y, z+1$; (vi) $-x+1, -y, -z+1$; (vii) $x-1, y, z$.