

Cs₁₀Ta_{29.27}O₇₈

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Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{Ta}-\text{O}) = 0.010$ Å; disorder in main residue; R factor = 0.033; wR factor = 0.083; data-to-parameter ratio = 12.8.

Single crystals of caesium tantalate(V), Cs₁₀Ta_{29.27}O₇₈, were obtained as a serendipitous product in a welded tantalum ampoule by a blank reaction of CsBr and bismuth subnitrate [Bi₅O(OH)₉(NO₃)₄] with the container material. The crystal structure of the title compound is made up of a three-dimensional framework constituted by two types of layers, *viz.* (Ta₆O₁₅)_{*n*} and (Ta₃O₉)_{*n*}, parallel to (001), which are linked together by TaO₆ octahedra ($3m$. symmetry) along [001]. This framework has cavities where three independent Cs⁺ ions ($3m$. and $\bar{6}m2$ symmetry, respectively) are located. The compound reveals a Ta deficiency at one trigonal prismatic coordinated site ($\bar{6}m2$ symmetry). The composition of the title compound was verified by energy-dispersive X-ray analysis of single crystals.

Related literature

For a previous powder diffraction study of Cs₁₀Ta_{29.27}O₇₈, see: Michel *et al.* (1978). For an isotopic compound, see: Haddad & Jouini (1997). For general background and related structures, see: du Boulay *et al.* (2003); Magnéli (1953); Marini *et al.* (1979); Serafin & Hoppe (1982).

Experimental

Crystal data

| | |
|--|---|
| Cs ₁₀ Ta _{29.27} O ₇₈ | $Z = 1$ |
| $M_r = 7873.51$ | Mo $K\alpha$ radiation |
| Hexagonal, $P6_3/mmc$ | $\mu = 49.96 \text{ mm}^{-1}$ |
| $a = 7.5170$ (11) Å | $T = 294$ (2) K |
| $c = 36.340$ (7) Å | $0.03 \times 0.02 \times 0.01 \text{ mm}$ |
| $V = 1778.3$ (5) Å ³ | |

Data collection

| | |
|---|---------------------------------------|
| Stoe IPDS-I diffractometer | 14043 measured reflections |
| Absorption correction: numerical (<i>X-SHAPE</i> ; Stoe & Cie, 1999) | 855 independent reflections |
| $T_{\min} = 0.218$, $T_{\max} = 0.607$ | 587 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.119$ |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.033$ | 67 parameters |
| $wR(F^2) = 0.083$ | $\Delta\rho_{\max} = 1.54 \text{ e \AA}^{-3}$ |
| $S = 0.89$ | $\Delta\rho_{\min} = -3.28 \text{ e \AA}^{-3}$ |
| 855 reflections | |

Data collection: *X-Area* (Stoe & Cie, 2002); cell refinement: *X-Area*; data reduction: *X-Area*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2217).

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supplementary materials

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Cs₁₀Ta_{29.27}O₇₈

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Comment

The title compound has a three-dimensional framework, constituted by two types of layers, (Ta₆O₁₅)_n (Fig. 1, green) and (Ta₃O₉)_n (Fig. 2, blue), parallel to (001). These layers are linked together along [001], according to the sequence (Ta₆O₁₅)_n-TaO₆-(Ta₃O₉)_n-(Ta₃O₉)_n-TaO₆, by sharing corners of TaO₆ octahedra (red, Fig. 3). The tantalum atom with deficient occupation is located in a site with trigonal-prismatic coordinated sites (yellow), between two Ta₃O₉ units belonging to two neighboring (Ta₃O₉)_n layers. This framework has cavities which communicate with interconnected channels, parallel to [100]. Cs⁺ ions (black) are located in these cavities. Geometric parameters of the title compound are in the usual ranges. Based on a previous powder diffraction study of Cs₁₀Ta_{29.27}O₇₈ reported by Michel *et al.* (1978), an additional Ta site was found, but was not observed in the current re-investigation. The closely related structure of Tl₁₀Nb_{29.2}O₇₈ was also reported (Marini *et al.*, 1979) with an additional Nb site with too short interatomic distances between the Nb atoms.

The title compound crystallizes isotypically with Rb₅VONb₁₄O₃₈ (Haddad & Jouini, 1997), in which the vanadium atom occupies the trigonal-prismatic Ta deficiency site of the title compound. The related compound Cs₃Ta₅O₁₄ was first investigated by powder diffraction studies by Serafin & Hoppe (1982) and was later re-investigated on the basis of single-crystal X-ray diffraction by du Boulay *et al.* (2003). An overview on the related hexagonal tungsten bronzes of potassium, rubidium and caesium was presented by Magnéli (1953).

Experimental

The title compound was obtained as a serendipitous product by the reaction of CsBr and bismuth subnitrate (Bi₅O(OH)₉(NO₃)₄, 98%, Sigma-Aldrich) with the tantalum container material. It was synthesized under argon at temperatures of 1523 K in a welded tantalum ampoule. The air stable title compound crystallizes in brown rods. The chemical composition of the single-crystal was confirmed by energy-dispersive X-ray (EDX) analysis which revealed no impurity elements.

Refinement

The site occupation factor (s.o.f.) of the Ta-deficient Ta4 site was refined freely. The maximum residual electron density lies 0.95 Å from O1 and the minimum residual electron density lies at the position of the Cs1 atom.

Figures

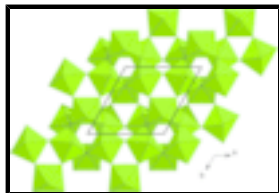


Fig. 1. View along [001] on the (Ta₆O₁₅)_n layer.

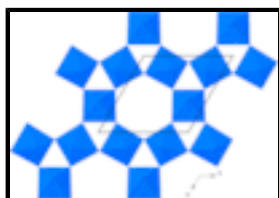


Fig. 2. View along [001] on the (Ta₃O₉)_n layer.

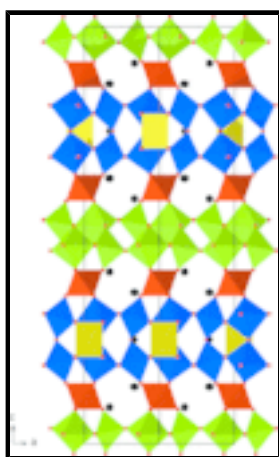


Fig. 3. View along [010] on the layers of the title compound connected *via* TaO₆ octahedra. Displacement ellipsoids are drawn at the 50% probability level.

caesium tantalate(V)

Crystal data

Cs₁₀Ta_{29.27}O₇₈

M_r = 7873.51

Hexagonal, *P*6₃/*mmc*

Hall symbol: -P 6c 2c

a = 7.5170 (11) Å

b = 7.5170 (11) Å

c = 36.340 (7) Å

α = 90°

β = 90°

γ = 120°

V = 1778.3 (5) Å³

Z = 1

*F*₀₀₀ = 3310.4

D_x = 7.352 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 1275 reflections

θ = 2.6–31.6°

μ = 49.96 mm⁻¹

T = 294 (2) K

Rod, brown

0.03 × 0.02 × 0.01 mm

Data collection

Stoe IPDS-I

855 independent reflections

diffractometer
 Radiation source: fine-focus sealed tube 587 reflections with $I > 2\sigma(I)$
 Monochromator: graphite $R_{\text{int}} = 0.119$
 $T = 294(2)$ K $\theta_{\text{max}} = 27.5^\circ$
 ω scans $\theta_{\text{min}} = 3.1^\circ$
 Absorption correction: numerical $h = -9 \rightarrow 9$
 (X-SHAPE; Stoe & Cie, 1999) $k = -9 \rightarrow 9$
 $T_{\text{min}} = 0.218$, $T_{\text{max}} = 0.607$ $l = -46 \rightarrow 46$
 14043 measured reflections

Refinement

Refinement on F^2 Primary atom site location: structure-invariant direct methods
 Least-squares matrix: full Secondary atom site location: difference Fourier map
 $R[F^2 > 2\sigma(F^2)] = 0.033$ $w = 1/[\sigma^2(F_o^2) + (0.0516P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.083$ $(\Delta/\sigma)_{\text{max}} < 0.001$
 $S = 0.89$ $\Delta\rho_{\text{max}} = 1.54 \text{ e } \text{\AA}^{-3}$
 855 reflections $\Delta\rho_{\text{min}} = -3.28 \text{ e } \text{\AA}^{-3}$
 67 parameters Extinction correction: none

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)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|--------------|--------------|---------------|----------------------------------|------------|
| Ta1 | 0.0000 | 0.0000 | 0.11749 (3) | 0.0166 (2) | |
| Ta2 | 0.33551 (10) | 0.16775 (5) | 0.034126 (15) | 0.01525 (19) | |
| Ta3 | 0.17146 (6) | 0.34292 (11) | 0.196383 (17) | 0.0204 (2) | |
| Ta4 | 0.0000 | 0.0000 | 0.2500 | 0.0163 (8) | 0.633 (10) |
| O1 | 0.0814 (19) | 0.5407 (9) | 0.1881 (4) | 0.021 (2) | |
| O2 | 0.5486 (9) | 0.4514 (9) | 0.0368 (3) | 0.019 (2) | |
| O3 | 0.1256 (9) | 0.2511 (18) | 0.1456 (3) | 0.022 (2) | |
| O4 | 0.2470 (17) | 0.1235 (8) | 0.0825 (3) | 0.017 (2) | |
| O5 | 0.1410 (8) | -0.1410 (8) | 0.0233 (3) | 0.012 (2) | |
| O6 | 0.2379 (18) | 0.1190 (9) | 0.2082 (3) | 0.019 (2) | |
| O7 | 0.1878 (15) | 0.376 (3) | 0.2500 | 0.023 (4) | |

supplementary materials

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|-----|--------|--------|-------------|------------|
| Cs1 | 0.6667 | 0.3333 | 0.2500 | 0.0337 (6) |
| Cs2 | 0.3333 | 0.6667 | 0.08755 (7) | 0.0459 (6) |
| Cs3 | 0.6667 | 0.3333 | 0.13681 (8) | 0.0564 (7) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|---------------|---------------|
| Ta1 | 0.0158 (3) | 0.0158 (3) | 0.0180 (5) | 0.00791 (16) | 0.000 | 0.000 |
| Ta2 | 0.0141 (3) | 0.0144 (3) | 0.0173 (3) | 0.00703 (15) | -0.0001 (2) | -0.00005 (11) |
| Ta3 | 0.0181 (3) | 0.0217 (4) | 0.0226 (4) | 0.01083 (19) | -0.00299 (13) | -0.0060 (3) |
| Ta4 | 0.0151 (10) | 0.0151 (10) | 0.0188 (13) | 0.0075 (5) | 0.000 | 0.000 |
| O1 | 0.019 (5) | 0.014 (4) | 0.031 (6) | 0.010 (3) | -0.001 (5) | 0.000 (2) |
| O2 | 0.020 (4) | 0.020 (4) | 0.022 (5) | 0.013 (5) | 0.002 (2) | -0.002 (2) |
| O3 | 0.025 (5) | 0.019 (6) | 0.020 (5) | 0.010 (3) | 0.000 (2) | 0.000 (4) |
| O4 | 0.016 (5) | 0.016 (4) | 0.019 (5) | 0.008 (3) | 0.007 (4) | 0.004 (2) |
| O5 | 0.015 (4) | 0.015 (4) | 0.002 (4) | 0.005 (4) | -0.0019 (19) | 0.0019 (19) |
| O6 | 0.016 (5) | 0.013 (4) | 0.028 (6) | 0.008 (3) | 0.000 (4) | 0.000 (2) |
| O7 | 0.021 (6) | 0.038 (11) | 0.015 (7) | 0.019 (5) | 0.000 | 0.000 |
| Cs1 | 0.0317 (9) | 0.0317 (9) | 0.0377 (15) | 0.0159 (5) | 0.000 | 0.000 |
| Cs2 | 0.0443 (8) | 0.0443 (8) | 0.0493 (15) | 0.0221 (4) | 0.000 | 0.000 |
| Cs3 | 0.0626 (11) | 0.0626 (11) | 0.0441 (14) | 0.0313 (6) | 0.000 | 0.000 |

Geometric parameters (\AA , $^\circ$)

| | | | |
|---------------------------------------|-------------|---------------------------|------------|
| Ta1—O3 | 1.928 (12) | Ta3—O7 | 1.960 (2) |
| Ta1—O3 ⁱ | 1.928 (12) | Ta3—O6 ⁱⁱ | 2.028 (12) |
| Ta1—O3 ⁱⁱ | 1.928 (12) | Ta3—O6 | 2.027 (10) |
| Ta1—O4 ⁱ | 2.050 (11) | Ta3—Ta4 | 2.9631 (8) |
| Ta1—O4 ⁱⁱ | 2.050 (11) | Ta4—O6 ⁱ | 2.170 (12) |
| Ta1—O4 | 2.050 (11) | Ta4—O6 ⁱⁱ | 2.170 (12) |
| Ta2—O4 | 1.850 (11) | Ta4—O6 ^{vii} | 2.170 (12) |
| Ta2—O2 | 1.925 (7) | Ta4—O6 | 2.170 (12) |
| Ta2—O2 ⁱⁱⁱ | 1.925 (8) | Ta4—O6 ^{viii} | 2.170 (12) |
| Ta2—O5 ⁱⁱ | 2.070 (4) | Ta4—O6 ^{ix} | 2.170 (12) |
| Ta2—O5 | 2.070 (4) | Ta4—O7 ⁱⁱ | 2.45 (2) |
| Ta2—O5 ^{iv} | 2.114 (10) | Ta4—O7 | 2.45 (2) |
| Ta2—Ta2 ^v | 3.3049 (10) | Ta4—O7 ^{ix} | 2.446 (19) |
| Ta2—Ta2 ^{iv} | 3.3049 (10) | Ta4—Ta3 ⁱⁱ | 2.9631 (8) |
| Ta3—O3 | 1.940 (12) | Ta4—Ta3 ⁱ | 2.9631 (8) |
| Ta3—O1 | 1.941 (12) | Ta4—Ta3 ^{vii} | 2.9631 (8) |
| Ta3—O1 ^{vi} | 1.941 (12) | | |
| O3—Ta1—O3 ⁱ | 94.5 (5) | O3—Ta3—Ta4 | 113.2 (4) |
| O3—Ta1—O3 ⁱⁱ | 94.5 (5) | O1—Ta3—Ta4 | 127.0 (4) |
| O3 ⁱ —Ta1—O3 ⁱⁱ | 94.5 (5) | O1 ^{vi} —Ta3—Ta4 | 127.0 (4) |
| O3—Ta1—O4 ⁱ | 173.7 (5) | O7—Ta3—Ta4 | 55.1 (6) |

| | | | |
|--|------------|---|--------------|
| O3 ⁱ —Ta1—O4 ⁱ | 89.8 (3) | O6 ⁱⁱ —Ta3—Ta4 | 47.1 (3) |
| O3 ⁱⁱ —Ta1—O4 ⁱ | 89.8 (3) | O6—Ta3—Ta4 | 47.1 (3) |
| O3—Ta1—O4 ⁱⁱ | 89.8 (3) | O6 ⁱ —Ta4—O6 ⁱⁱ | 76.4 (5) |
| O3 ⁱ —Ta1—O4 ⁱⁱ | 173.7 (5) | O6 ⁱ —Ta4—O6 ^{vii} | 138.2 (2) |
| O3 ⁱⁱ —Ta1—O4 ⁱⁱ | 89.8 (3) | O6 ⁱⁱ —Ta4—O6 ^{vii} | 138.2 (2) |
| O4 ⁱ —Ta1—O4 ⁱⁱ | 85.6 (5) | O6 ⁱ —Ta4—O6 | 76.4 (5) |
| O3—Ta1—O4 | 89.8 (3) | O6 ⁱⁱ —Ta4—O6 | 76.4 (5) |
| O3 ⁱ —Ta1—O4 | 89.8 (3) | O6 ^{vii} —Ta4—O6 | 88.9 (6) |
| O3 ⁱⁱ —Ta1—O4 | 173.7 (5) | O6 ⁱ —Ta4—O6 ^{viii} | 138.2 (2) |
| O4 ⁱ —Ta1—O4 | 85.6 (5) | O6 ⁱⁱ —Ta4—O6 ^{viii} | 88.9 (6) |
| O4 ⁱⁱ —Ta1—O4 | 85.6 (5) | O6 ^{vii} —Ta4—O6 ^{viii} | 76.4 (5) |
| O4—Ta2—O2 | 100.2 (4) | O6—Ta4—O6 ^{viii} | 138.2 (2) |
| O4—Ta2—O2 ⁱⁱⁱ | 100.2 (4) | O6 ⁱ —Ta4—O6 ^{ix} | 88.9 (6) |
| O2—Ta2—O2 ⁱⁱⁱ | 87.5 (7) | O6 ⁱⁱ —Ta4—O6 ^{ix} | 138.2 (2) |
| O4—Ta2—O5 ⁱⁱ | 89.5 (4) | O6 ^{vii} —Ta4—O6 ^{ix} | 76.4 (5) |
| O2—Ta2—O5 ⁱⁱ | 85.4 (4) | O6—Ta4—O6 ^{ix} | 138.2 (2) |
| O2 ⁱⁱⁱ —Ta2—O5 ⁱⁱ | 168.9 (4) | O6 ^{viii} —Ta4—O6 ^{ix} | 76.4 (5) |
| O4—Ta2—O5 | 89.5 (4) | O6 ⁱ —Ta4—O7 ⁱⁱ | 69.09 (12) |
| O2—Ta2—O5 | 168.9 (4) | O6 ⁱⁱ —Ta4—O7 ⁱⁱ | 69.09 (12) |
| O2 ⁱⁱⁱ —Ta2—O5 | 85.4 (4) | O6 ^{vii} —Ta4—O7 ⁱⁱ | 135.5 (3) |
| O5 ⁱⁱ —Ta2—O5 | 100.3 (6) | O6—Ta4—O7 ⁱⁱ | 135.5 (3) |
| O4—Ta2—O5 ^{iv} | 152.4 (5) | O6 ^{viii} —Ta4—O7 ⁱⁱ | 69.09 (12) |
| O2—Ta2—O5 ^{iv} | 99.7 (4) | O6 ^{ix} —Ta4—O7 ⁱⁱ | 69.09 (12) |
| O2 ⁱⁱⁱ —Ta2—O5 ^{iv} | 99.7 (4) | O6 ⁱ —Ta4—O7 | 135.5 (3) |
| O5 ⁱⁱ —Ta2—O5 ^{iv} | 73.2 (4) | O6 ⁱⁱ —Ta4—O7 | 69.09 (12) |
| O5—Ta2—O5 ^{iv} | 73.2 (4) | O6 ^{vii} —Ta4—O7 | 69.09 (12) |
| O4—Ta2—Ta2 ^v | 127.6 (2) | O6—Ta4—O7 | 69.09 (12) |
| O2—Ta2—Ta2 ^v | 132.2 (3) | O6 ^{viii} —Ta4—O7 | 69.09 (12) |
| O2 ⁱⁱⁱ —Ta2—Ta2 ^v | 83.1 (3) | O6 ^{ix} —Ta4—O7 | 135.5 (3) |
| O5 ⁱⁱ —Ta2—Ta2 ^v | 95.4 (3) | O7 ⁱⁱ —Ta4—O7 | 120.000 (1) |
| O5—Ta2—Ta2 ^v | 38.3 (3) | O6 ⁱ —Ta4—O7 ^{ix} | 69.09 (12) |
| O5 ^{iv} —Ta2—Ta2 ^v | 37.37 (10) | O6 ⁱⁱ —Ta4—O7 ^{ix} | 135.5 (3) |
| O4—Ta2—Ta2 ^{iv} | 127.6 (2) | O6 ^{vii} —Ta4—O7 ^{ix} | 69.09 (12) |
| O2—Ta2—Ta2 ^{iv} | 83.1 (3) | O6—Ta4—O7 ^{ix} | 69.09 (12) |
| O2 ⁱⁱⁱ —Ta2—Ta2 ^{iv} | 132.2 (3) | O6 ^{viii} —Ta4—O7 ^{ix} | 135.5 (3) |
| O5 ⁱⁱ —Ta2—Ta2 ^{iv} | 38.3 (3) | O6 ^{ix} —Ta4—O7 ^{ix} | 69.09 (12) |
| O5—Ta2—Ta2 ^{iv} | 95.4 (3) | O7 ⁱⁱ —Ta4—O7 ^{ix} | 120.000 (1) |
| O5 ^{iv} —Ta2—Ta2 ^{iv} | 37.37 (10) | O7—Ta4—O7 ^{ix} | 120.000 (2) |
| Ta2 ^v —Ta2—Ta2 ^{iv} | 69.83 (3) | Ta3 ⁱⁱ —Ta4—Ta3 ^{vii} | 135.741 (10) |
| O3—Ta3—O1 | 93.3 (4) | Ta3 ⁱ —Ta4—Ta3 ^{vii} | 135.741 (10) |
| O3—Ta3—O1 ^{vi} | 93.3 (5) | Ta3—O1—Ta3 ^x | 140.3 (7) |

supplementary materials

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|--|-----------|---------------------------------------|------------|
| O1—Ta3—O1 ^{vi} | 94.1 (7) | Ta2—O2—Ta2 ^{xi} | 151.8 (7) |
| O3—Ta3—O7 | 168.3 (7) | Ta1—O3—Ta3 | 139.9 (7) |
| O1—Ta3—O7 | 94.7 (5) | Ta2—O4—Ta1 | 146.5 (7) |
| O1 ^{vi} —Ta3—O7 | 94.7 (5) | Ta2 ⁱ —O5—Ta2 | 132.0 (6) |
| O3—Ta3—O6 ⁱⁱ | 88.8 (4) | Ta2 ⁱ —O5—Ta2 ^v | 104.3 (3) |
| O1—Ta3—O6 ⁱⁱ | 91.5 (5) | Ta2—O5—Ta2 ^v | 104.3 (3) |
| O1 ^{vi} —Ta3—O6 ⁱⁱ | 173.9 (5) | Ta3 ⁱ —O6—Ta3 | 145.0 (6) |
| O7—Ta3—O6 ⁱⁱ | 82.4 (6) | Ta3 ⁱ —O6—Ta4 | 89.8 (3) |
| O3—Ta3—O6 | 88.8 (4) | Ta3—O6—Ta4 | 89.8 (3) |
| O1—Ta3—O6 | 173.9 (5) | Ta3—O7—Ta3 ^{vii} | 167.5 (11) |
| O1 ^{vi} —Ta3—O6 | 91.5 (5) | Ta3—O7—Ta4 | 83.8 (6) |
| O7—Ta3—O6 | 82.4 (5) | Ta3 ^{vii} —O7—Ta4 | 83.8 (6) |
| O6 ⁱⁱ —Ta3—O6 | 82.9 (6) | | |

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

Fig. 1

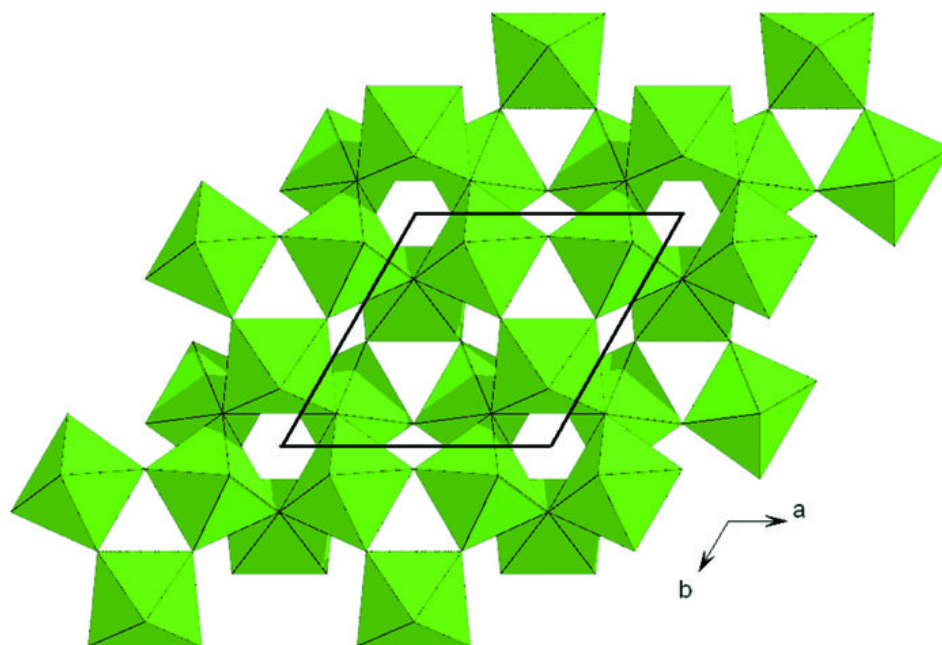


Fig. 2

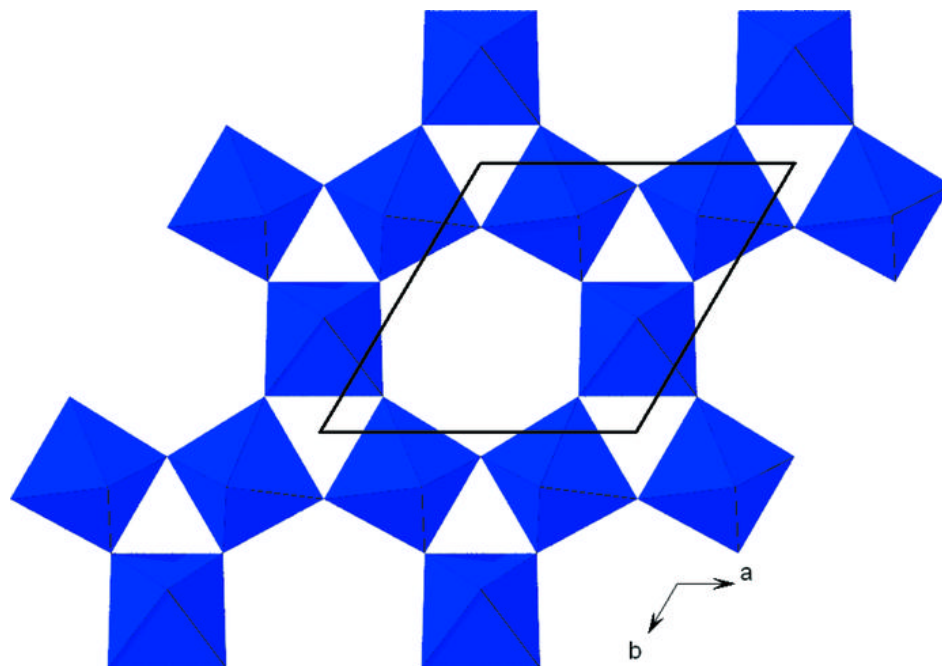


Fig. 3

