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Supporting information for article:

Single crystals of the filled Ti₂N-type η-phase Ti₃Zn₃O_x (x = 1.07 and 1.23) prepared using a Bi flux

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Data collection: [APEX3 v2016.9-0 \(Bruker AXS\)](#); cell refinement: [APEX3 v2016.9-0 \(Bruker AXS\)](#); data reduction: [APEX3 v2016.9-0 \(Bruker AXS\)](#); program(s) used to solve structure: [APEX3 v2016.9-0 \(Bruker AXS\)](#); program(s) used to refine structure: [SHELXL2014/7 \(Sheldrick, 2014\)](#); molecular graphics: [VESTA v2.1.6 \(Momma & Izumi, 2011\)](#)

Ti₃Zn₃O_{1.03}

Crystal data

| | |
|---|---|
| Ti ₃ Zn ₃ O _{1.03} | $D_x = 6.227 \text{ Mg m}^{-3}$ |
| $M_r = 356.37$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Cubic, $Fd\bar{3}m$ | Cell parameters from 793 reflections |
| | $\theta = 3.1\text{--}38.7^\circ$ |
| $a = 11.4990 (2) \text{ \AA}$ | $\mu = 24.41 \text{ mm}^{-1}$ |
| $V = 1520.48 (8) \text{ \AA}^3$ | $T = 302 \text{ K}$ |
| $Z = 16$ | Granule, black |
| $F(000) = 2628$ | $0.08 \times 0.07 \times 0.04 \text{ mm}$ |

Data collection

| | |
|---|---|
| Bruker D8 goniometer diffractometer | 210 independent reflections |
| Radiation source: micro focus sealed tube | 199 reflections with $I > 2\sigma(I)$ |
| Detector resolution: $7.4074 \text{ pixels mm}^{-1}$ | $R_{\text{int}} = 0.030$ |
| ω, φ scans | $\theta_{\text{max}} = 36.1^\circ, \theta_{\text{min}} = 3.1^\circ$ |
| Absorption correction: multi-scan SADABS2016/2 - Bruker AXS area detector scaling and absorption correction | $h = -19 \rightarrow 19$ |
| $T_{\text{min}} = 0.35, T_{\text{max}} = 0.42$ | $k = -19 \rightarrow 19$ |
| 9213 measured reflections | $l = -19 \rightarrow 18$ |

Refinement

| | |
|---------------------------------|---|
| Refinement on F^2 | $w = 1/[\sigma^2(F_o^2) + (0.0064P)^2 + 2.5084P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| Least-squares matrix: full | $(\Delta/\sigma)_{\max} = 0.001$ |
| $R[F^2 > 2\sigma(F^2)] = 0.008$ | $\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$ |
| $wR(F^2) = 0.019$ | $\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$ |
| $S = 1.24$ | Extinction correction: <i>SHELXL2014/7</i> (Sheldrick 2014) |
| 210 reflections | Extinction coefficient: 0.00058 (3) |
| 15 parameters | $w = 1/[\sigma^2(F_o^2) + (0.0064P)^2 + 2.5084P]$ where $P = (F_o^2 + 2F_c^2)/3$ |

Special details

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

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|-------------|-------------|-------------|----------------------------------|------------|
| Ti1 | 0.30578 (2) | 0.125 | 0.125 | 0.00455 (6) | |
| Zn1 | 0.29059 (2) | 0.29059 (2) | 0.29059 (2) | 0.00551 (6) | |
| Zn2 | 0.5 | 0.5 | 0.5 | 0.00707 (7) | |
| O1 | 0 | 0 | 0 | 0.0051 (3) | |
| O2 | 0.125 | 0.125 | 0.125 | 0.010 (9) | 0.071 (12) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|-------------|-------------|--------------|--------------|--------------|
| Ti1 | 0.00580 (10) | 0.00392 (7) | 0.00392 (7) | 0 | 0 | 0.00003 (7) |
| Zn1 | 0.00551 (6) | 0.00551 (6) | 0.00551 (6) | -0.00044 (4) | -0.00044 (4) | -0.00044 (4) |
| Zn2 | 0.00707 (7) | 0.00707 (7) | 0.00707 (7) | -0.00147 (5) | -0.00147 (5) | -0.00147 (5) |
| O1 | 0.0051 (3) | 0.0051 (3) | 0.0051 (3) | -0.0003 (3) | -0.0003 (3) | -0.0003 (3) |
| O2 | 0.010 (9) | 0.010 (9) | 0.010 (9) | 0 | 0 | 0 |

Geometric parameters (Å, °)

| | | | |
|---------------------------------------|--------------|---|--------------|
| Ti1—O2 | 2.0788 (2) | Zn2—Zn1 ^{xvi} | 2.4968 (1) |
| Ti1—O1 ⁱ | 2.1316 (1) | Zn2—Zn1 ^{viii} | 2.4968 (1) |
| Ti1—O1 ⁱⁱ | 2.1316 (1) | Zn2—Zn1 ^{xvii} | 2.4968 (1) |
| Ti1—Zn1 | 2.6985 (2) | Zn2—Zn1 ^{xi} | 2.4968 (1) |
| Ti1—Zn1 ⁱⁱⁱ | 2.6985 (2) | Zn2—Zn1 ^{xviii} | 2.4968 (1) |
| Ti1—Ti1 ^{iv} | 2.9398 (3) | Zn2—Zn1 ^{xii} | 2.4968 (1) |
| Ti1—Ti1 ^v | 2.9398 (3) | Zn2—Ti1 ^{xix} | 3.0199 (2) |
| Ti1—Ti1 ^{vi} | 2.9398 (3) | Zn2—Ti1 ^{xx} | 3.0199 (2) |
| Ti1—Ti1 ^{vii} | 2.9398 (3) | Zn2—Ti1 ^{xxi} | 3.0199 (2) |
| Ti1—Zn2 ^{viii} | 3.0199 (2) | Zn2—Ti1 ^{xxii} | 3.0199 (2) |
| Ti1—Zn2 ^{ix} | 3.0199 (2) | Zn2—Ti1 ^{xxiii} | 3.0199 (2) |
| Ti1—Zn1 ^x | 3.0290 (2) | Zn2—Ti1 ^{xxiv} | 3.0199 (2) |
| Zn1—Zn2 ^{viii} | 2.4968 (1) | O1—Ti1 ^{xxv} | 2.1316 (1) |
| Zn1—Zn2 ^{xi} | 2.4968 (1) | O1—Ti1 ^{iv} | 2.1316 (1) |
| Zn1—Zn2 ^{xii} | 2.4968 (1) | O1—Ti1 ⁱⁱ | 2.1316 (1) |
| Zn1—Ti1 ^{vii} | 2.6985 (2) | O1—Ti1 ^v | 2.1316 (1) |
| Zn1—Ti1 ^{vi} | 2.6985 (2) | O1—Ti1 ^{xxvi} | 2.1316 (1) |
| Zn1—Zn1 ^{viii} | 2.7454 (3) | O1—Ti1 ^{xxvii} | 2.1316 (1) |
| Zn1—Zn1 ^{xii} | 2.7454 (3) | O2—Ti1 ^{iv} | 2.0788 (2) |
| Zn1—Zn1 ^{xi} | 2.7454 (3) | O2—Ti1 ^{vi} | 2.0788 (2) |
| Zn1—Ti1 ^{xiii} | 3.0290 (2) | O2—Ti1 ⁱⁱ | 2.0788 (2) |
| Zn1—Ti1 ^{xiv} | 3.0290 (2) | O2—Ti1 ^{vii} | 2.0788 (2) |
| Zn1—Ti1 ^{xv} | 3.0290 (2) | O2—Ti1 ^v | 2.0788 (2) |
| O2—Ti1—O1 ⁱ | 72.487 (6) | Ti1 ^{vii} —Zn1—Ti1 ^{xiv} | 120.660 (10) |
| O2—Ti1—O1 ⁱⁱ | 72.487 (6) | Ti1 ^{vi} —Zn1—Ti1 ^{xiv} | 64.936 (2) |
| O1 ⁱ —Ti1—O1 ⁱⁱ | 144.974 (12) | Ti1—Zn1—Ti1 ^{xiv} | 64.936 (2) |
| O2—Ti1—Zn1 | 86.288 (6) | Zn1 ^{viii} —Zn1—Ti1 ^{xiv} | 113.811 (4) |
| O1 ⁱ —Ti1—Zn1 | 88.884 (2) | Zn1 ^{xii} —Zn1—Ti1 ^{xiv} | 113.811 (4) |
| O1 ⁱⁱ —Ti1—Zn1 | 88.884 (2) | Zn1 ^{xi} —Zn1—Ti1 ^{xiv} | 63.051 (4) |

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|--|--------------|---|--------------|
| O2—Ti1—Zn1 ⁱⁱⁱ | 86.288 (6) | Ti1 ^{xiii} —Zn1—Ti1 ^{xiv} | 117.945 (2) |
| O1 ⁱ —Ti1—Zn1 ⁱⁱⁱ | 88.884 (2) | Zn2 ^{viii} —Zn1—Ti1 ^{xv} | 168.380 (8) |
| O1 ⁱⁱ —Ti1—Zn1 ⁱⁱⁱ | 88.884 (2) | Zn2 ^{xi} —Zn1—Ti1 ^{xv} | 65.4310 (10) |
| Zn1—Ti1—Zn1 ⁱⁱⁱ | 172.576 (12) | Zn2 ^{xii} —Zn1—Ti1 ^{xv} | 65.4310 (10) |
| O2—Ti1—Ti1 ^{iv} | 45.0 | Ti1 ^{vii} —Zn1—Ti1 ^{xv} | 64.936 (2) |
| O1 ⁱ —Ti1—Ti1 ^{iv} | 105.310 (5) | Ti1 ^{vi} —Zn1—Ti1 ^{xv} | 64.936 (2) |
| O1 ⁱⁱ —Ti1—Ti1 ^{iv} | 46.401 (4) | Ti1—Zn1—Ti1 ^{xv} | 120.661 (10) |
| Zn1—Ti1—Ti1 ^{iv} | 116.947 (5) | Zn1 ^{viii} —Zn1—Ti1 ^{xv} | 63.051 (4) |
| Zn1 ⁱⁱⁱ —Ti1—Ti1 ^{iv} | 56.994 (5) | Zn1 ^{xii} —Zn1—Ti1 ^{xv} | 113.811 (4) |
| O2—Ti1—Ti1 ^v | 45.0 | Zn1 ^{xi} —Zn1—Ti1 ^{xv} | 113.811 (4) |
| O1 ⁱ —Ti1—Ti1 ^v | 46.401 (4) | Ti1 ^{xiii} —Zn1—Ti1 ^{xv} | 117.945 (2) |
| O1 ⁱⁱ —Ti1—Ti1 ^v | 105.310 (5) | Ti1 ^{xiv} —Zn1—Ti1 ^{xv} | 117.945 (2) |
| Zn1—Ti1—Ti1 ^v | 116.947 (5) | Zn1 ^{xvi} —Zn2—Zn1 ^{viii} | 180.0 |
| Zn1 ⁱⁱⁱ —Ti1—Ti1 ^v | 56.994 (5) | Zn1 ^{xvi} —Zn2—Zn1 ^{xvii} | 66.703 (7) |
| Ti1 ^{iv} —Ti1—Ti1 ^v | 60.0 | Zn1 ^{viii} —Zn2—Zn1 ^{xvii} | 113.297 (7) |
| O2—Ti1—Ti1 ^{vi} | 45.0 | Zn1 ^{xvi} —Zn2—Zn1 ^{xi} | 113.297 (7) |
| O1 ⁱ —Ti1—Ti1 ^{vi} | 46.401 (4) | Zn1 ^{viii} —Zn2—Zn1 ^{xi} | 66.703 (7) |
| O1 ⁱⁱ —Ti1—Ti1 ^{vi} | 105.310 (5) | Zn1 ^{xvii} —Zn2—Zn1 ^{xi} | 180.0 |
| Zn1—Ti1—Ti1 ^{vi} | 56.994 (5) | Zn1 ^{xvi} —Zn2—Zn1 ^{xviii} | 66.703 (7) |
| Zn1 ⁱⁱⁱ —Ti1—Ti1 ^{vi} | 116.947 (5) | Zn1 ^{viii} —Zn2—Zn1 ^{xviii} | 113.297 (7) |
| Ti1 ^{iv} —Ti1—Ti1 ^{vi} | 90.0 | Zn1 ^{xvii} —Zn2—Zn1 ^{xviii} | 66.703 (7) |
| Ti1 ^v —Ti1—Ti1 ^{vi} | 60.0 | Zn1 ^{xi} —Zn2—Zn1 ^{xviii} | 113.297 (7) |
| O2—Ti1—Ti1 ^{vii} | 45.0 | Zn1 ^{xvi} —Zn2—Zn1 ^{xii} | 113.297 (7) |
| O1 ⁱ —Ti1—Ti1 ^{vii} | 105.310 (5) | Zn1 ^{viii} —Zn2—Zn1 ^{xii} | 66.703 (7) |
| O1 ⁱⁱ —Ti1—Ti1 ^{vii} | 46.401 (4) | Zn1 ^{xvii} —Zn2—Zn1 ^{xii} | 113.297 (7) |
| Zn1—Ti1—Ti1 ^{vii} | 56.994 (5) | Zn1 ^{xi} —Zn2—Zn1 ^{xii} | 66.703 (7) |
| Zn1 ⁱⁱⁱ —Ti1—Ti1 ^{vii} | 116.947 (5) | Zn1 ^{xviii} —Zn2—Zn1 ^{xii} | 180.0 |
| Ti1 ^{iv} —Ti1—Ti1 ^{vii} | 60.0 | Zn1 ^{xvi} —Zn2—Ti1 ^{xix} | 122.364 (5) |
| Ti1 ^v —Ti1—Ti1 ^{vii} | 90.0 | Zn1 ^{viii} —Zn2—Ti1 ^{xix} | 57.636 (5) |
| Ti1 ^{vi} —Ti1—Ti1 ^{vii} | 60.0 | Zn1 ^{xvii} —Zn2—Ti1 ^{xix} | 65.810 (3) |
| O2—Ti1—Zn2 ^{viii} | 137.692 (3) | Zn1 ^{xi} —Zn2—Ti1 ^{xix} | 114.190 (3) |
| O1 ⁱ —Ti1—Zn2 ^{viii} | 102.858 (4) | Zn1 ^{xviii} —Zn2—Ti1 ^{xix} | 65.810 (3) |

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| O1 ⁱⁱ —Ti1—Zn2 ^{viii} | 102.858 (4) | Zn1 ^{xii} —Zn2—Ti1 ^{xix} | 114.190 (3) |
| Zn1—Ti1—Zn2 ^{viii} | 51.404 (3) | Zn1 ^{xvi} —Zn2—Ti1 ^{xx} | 114.190 (3) |
| Zn1 ⁱⁱⁱ —Ti1—Zn2 ^{viii} | 136.020 (9) | Zn1 ^{viii} —Zn2—Ti1 ^{xx} | 65.810 (3) |
| Ti1 ^{iv} —Ti1—Zn2 ^{viii} | 149.2590 (10) | Zn1 ^{xvii} —Zn2—Ti1 ^{xx} | 114.190 (3) |
| Ti1 ^v —Ti1—Zn2 ^{viii} | 149.2590 (10) | Zn1 ^{xi} —Zn2—Ti1 ^{xx} | 65.810 (3) |
| Ti1 ^{vi} —Ti1—Zn2 ^{viii} | 100.741 (3) | Zn1 ^{xviii} —Zn2—Ti1 ^{xx} | 57.636 (5) |
| Ti1 ^{vii} —Ti1—Zn2 ^{viii} | 100.741 (3) | Zn1 ^{xii} —Zn2—Ti1 ^{xx} | 122.364 (5) |
| O2—Ti1—Zn2 ^{ix} | 137.692 (3) | Ti1 ^{xix} —Zn2—Ti1 ^{xx} | 61.4810 (10) |
| O1 ⁱ —Ti1—Zn2 ^{ix} | 102.858 (4) | Zn1 ^{xvi} —Zn2—Ti1 ^{xxi} | 65.810 (3) |
| O1 ⁱⁱ —Ti1—Zn2 ^{ix} | 102.858 (4) | Zn1 ^{viii} —Zn2—Ti1 ^{xxi} | 114.190 (3) |
| Zn1—Ti1—Zn2 ^{ix} | 136.020 (9) | Zn1 ^{xvii} —Zn2—Ti1 ^{xxi} | 65.810 (3) |
| Zn1 ⁱⁱⁱ —Ti1—Zn2 ^{ix} | 51.404 (3) | Zn1 ^{xi} —Zn2—Ti1 ^{xxi} | 114.190 (3) |
| Ti1 ^{iv} —Ti1—Zn2 ^{ix} | 100.741 (3) | Zn1 ^{xviii} —Zn2—Ti1 ^{xxi} | 122.364 (5) |
| Ti1 ^v —Ti1—Zn2 ^{ix} | 100.741 (3) | Zn1 ^{xii} —Zn2—Ti1 ^{xxi} | 57.636 (5) |
| Ti1 ^{vi} —Ti1—Zn2 ^{ix} | 149.2590 (10) | Ti1 ^{xix} —Zn2—Ti1 ^{xxi} | 118.5190 (10) |
| Ti1 ^{vii} —Ti1—Zn2 ^{ix} | 149.2590 (10) | Ti1 ^{xx} —Zn2—Ti1 ^{xxi} | 180.0 |
| Zn2 ^{viii} —Ti1—Zn2 ^{ix} | 84.616 (6) | Zn1 ^{xvi} —Zn2—Ti1 ^{xxii} | 114.190 (3) |
| O2—Ti1—Zn1 ^x | 153.051 (4) | Zn1 ^{viii} —Zn2—Ti1 ^{xxii} | 65.810 (3) |
| O1 ⁱ —Ti1—Zn1 ^x | 80.564 (5) | Zn1 ^{xvii} —Zn2—Ti1 ^{xxii} | 57.636 (5) |
| O1 ⁱⁱ —Ti1—Zn1 ^x | 134.462 (9) | Zn1 ^{xi} —Zn2—Ti1 ^{xxii} | 122.364 (5) |
| Zn1—Ti1—Zn1 ^x | 93.309 (5) | Zn1 ^{xviii} —Zn2—Ti1 ^{xxii} | 114.190 (3) |
| Zn1 ⁱⁱⁱ —Ti1—Zn1 ^x | 93.308 (5) | Zn1 ^{xii} —Zn2—Ti1 ^{xxii} | 65.810 (3) |
| Ti1 ^{iv} —Ti1—Zn1 ^x | 148.9730 (10) | Ti1 ^{xix} —Zn2—Ti1 ^{xxii} | 61.4810 (10) |
| Ti1 ^v —Ti1—Zn1 ^x | 113.812 (4) | Ti1 ^{xx} —Zn2—Ti1 ^{xxii} | 118.5190 (10) |
| Ti1 ^{vi} —Ti1—Zn1 ^x | 113.812 (4) | Ti1 ^{xxi} —Zn2—Ti1 ^{xxii} | 61.4810 (10) |
| Ti1 ^{vii} —Ti1—Zn1 ^x | 148.9730 (10) | Zn1 ^{xvi} —Zn2—Ti1 ^{xxiii} | 65.810 (3) |
| Zn2 ^{viii} —Ti1—Zn1 ^x | 48.759 (4) | Zn1 ^{viii} —Zn2—Ti1 ^{xxiii} | 114.190 (3) |
| Zn2 ^{ix} —Ti1—Zn1 ^x | 48.759 (4) | Zn1 ^{xvii} —Zn2—Ti1 ^{xxiii} | 122.364 (5) |
| Zn2 ^{viii} —Zn1—Zn2 ^{xi} | 109.002 (4) | Zn1 ^{xi} —Zn2—Ti1 ^{xxiii} | 57.636 (5) |
| Zn2 ^{viii} —Zn1—Zn2 ^{xii} | 109.002 (4) | Zn1 ^{xviii} —Zn2—Ti1 ^{xxiii} | 65.810 (3) |
| Zn2 ^{xi} —Zn1—Zn2 ^{xii} | 109.002 (4) | Zn1 ^{xii} —Zn2—Ti1 ^{xxiii} | 114.190 (3) |
| Zn2 ^{viii} —Zn1—Ti1 ^{vii} | 124.106 (4) | Ti1 ^{xix} —Zn2—Ti1 ^{xxiii} | 118.5190 (10) |

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| Zn2 ^{xi} —Zn1—Ti1 ^{vii} | 70.960 (5) | Ti1 ^{xx} —Zn2—Ti1 ^{xxiii} | 61.4810 (10) |
| Zn2 ^{xii} —Zn1—Ti1 ^{vii} | 124.106 (4) | Ti1 ^{xxi} —Zn2—Ti1 ^{xxiii} | 118.5190 (10) |
| Zn2 ^{viii} —Zn1—Ti1 ^{vi} | 124.106 (4) | Ti1 ^{xxii} —Zn2—Ti1 ^{xxiii} | 180.0 |
| Zn2 ^{xi} —Zn1—Ti1 ^{vi} | 124.106 (4) | Zn1 ^{xvi} —Zn2—Ti1 ^{xxiv} | 57.636 (5) |
| Zn2 ^{xii} —Zn1—Ti1 ^{vi} | 70.960 (5) | Zn1 ^{viii} —Zn2—Ti1 ^{xxiv} | 122.364 (5) |
| Ti1 ^{vii} —Zn1—Ti1 ^{vi} | 66.012 (9) | Zn1 ^{xvii} —Zn2—Ti1 ^{xxiv} | 114.190 (3) |
| Zn2 ^{viii} —Zn1—Ti1 | 70.960 (5) | Zn1 ^{xi} —Zn2—Ti1 ^{xxiv} | 65.810 (3) |
| Zn2 ^{xi} —Zn1—Ti1 | 124.106 (4) | Zn1 ^{xviii} —Zn2—Ti1 ^{xxiv} | 114.190 (3) |
| Zn2 ^{xii} —Zn1—Ti1 | 124.106 (4) | Zn1 ^{xii} —Zn2—Ti1 ^{xxiv} | 65.810 (3) |
| Ti1 ^{vii} —Zn1—Ti1 | 66.012 (9) | Ti1 ^{xix} —Zn2—Ti1 ^{xxiv} | 180.0 |
| Ti1 ^{vi} —Zn1—Ti1 | 66.012 (9) | Ti1 ^{xx} —Zn2—Ti1 ^{xxiv} | 118.5190 (10) |
| Zn2 ^{viii} —Zn1—Zn1 ^{viii} | 105.328 (4) | Ti1 ^{xxi} —Zn2—Ti1 ^{xxiv} | 61.4810 (10) |
| Zn2 ^{xi} —Zn1—Zn1 ^{viii} | 56.648 (3) | Ti1 ^{xxii} —Zn2—Ti1 ^{xxiv} | 118.5190 (10) |
| Zn2 ^{xii} —Zn1—Zn1 ^{viii} | 56.648 (3) | Ti1 ^{xxiii} —Zn2—Ti1 ^{xxiv} | 61.4810 (10) |
| Ti1 ^{vii} —Zn1—Zn1 ^{viii} | 116.948 (5) | Ti1 ^{xxv} —O1—Ti1 ^{iv} | 180.000 (12) |
| Ti1 ^{vi} —Zn1—Zn1 ^{viii} | 116.948 (5) | Ti1 ^{xxv} —O1—Ti1 ⁱⁱ | 92.803 (9) |
| Ti1—Zn1—Zn1 ^{viii} | 176.288 (6) | Ti1 ^{iv} —O1—Ti1 ⁱⁱ | 87.197 (9) |
| Zn2 ^{viii} —Zn1—Zn1 ^{xii} | 56.648 (3) | Ti1 ^{xxv} —O1—Ti1 ^v | 92.803 (9) |
| Zn2 ^{xi} —Zn1—Zn1 ^{xii} | 56.648 (3) | Ti1 ^{iv} —O1—Ti1 ^v | 87.197 (9) |
| Zn2 ^{xii} —Zn1—Zn1 ^{xii} | 105.328 (4) | Ti1 ⁱⁱ —O1—Ti1 ^v | 87.197 (9) |
| Ti1 ^{vii} —Zn1—Zn1 ^{xii} | 116.948 (5) | Ti1 ^{xxv} —O1—Ti1 ^{xxvi} | 87.197 (9) |
| Ti1 ^{vi} —Zn1—Zn1 ^{xii} | 176.288 (6) | Ti1 ^{iv} —O1—Ti1 ^{xxvi} | 92.803 (9) |
| Ti1—Zn1—Zn1 ^{xii} | 116.947 (5) | Ti1 ⁱⁱ —O1—Ti1 ^{xxvi} | 92.803 (9) |
| Zn1 ^{viii} —Zn1—Zn1 ^{xii} | 60.0 | Ti1 ^v —O1—Ti1 ^{xxvi} | 180.000 (12) |
| Zn2 ^{viii} —Zn1—Zn1 ^{xi} | 56.648 (3) | Ti1 ^{xxv} —O1—Ti1 ^{xxvii} | 87.197 (9) |
| Zn2 ^{xi} —Zn1—Zn1 ^{xi} | 105.328 (4) | Ti1 ^{iv} —O1—Ti1 ^{xxvii} | 92.803 (9) |
| Zn2 ^{xii} —Zn1—Zn1 ^{xi} | 56.648 (3) | Ti1 ⁱⁱ —O1—Ti1 ^{xxvii} | 180.000 (12) |
| Ti1 ^{vii} —Zn1—Zn1 ^{xi} | 176.288 (6) | Ti1 ^v —O1—Ti1 ^{xxvii} | 92.803 (9) |
| Ti1 ^{vi} —Zn1—Zn1 ^{xi} | 116.948 (5) | Ti1 ^{xxvi} —O1—Ti1 ^{xxvii} | 87.197 (9) |
| Ti1—Zn1—Zn1 ^{xi} | 116.947 (5) | Ti1 ^{iv} —O2—Ti1 ^{vi} | 180.0 |
| Zn1 ^{viii} —Zn1—Zn1 ^{xi} | 60.0 | Ti1 ^{iv} —O2—Ti1 ⁱⁱ | 90.0 |
| Zn1 ^{xii} —Zn1—Zn1 ^{xi} | 60.0 | Ti1 ^{vi} —O2—Ti1 ⁱⁱ | 90.0 |

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| Zn2 ^{viii} —Zn1—Ti1 ^{xiii} | 65.4310 (10) | Ti1 ^{iv} —O2—Ti1 ^{vii} | 90.0 |
| Zn2 ^{xi} —Zn1—Ti1 ^{xiii} | 65.4310 (10) | Ti1 ^{vi} —O2—Ti1 ^{vii} | 90.0 |
| Zn2 ^{xii} —Zn1—Ti1 ^{xiii} | 168.380 (8) | Ti1 ⁱⁱ —O2—Ti1 ^{vii} | 90.0 |
| Ti1 ^{vii} —Zn1—Ti1 ^{xiii} | 64.936 (2) | Ti1 ^{iv} —O2—Ti1 ^v | 90.0 |
| Ti1 ^{vi} —Zn1—Ti1 ^{xiii} | 120.660 (10) | Ti1 ^{vi} —O2—Ti1 ^v | 90.0 |
| Ti1—Zn1—Ti1 ^{xiii} | 64.936 (2) | Ti1 ⁱⁱ —O2—Ti1 ^v | 90.0 |
| Zn1 ^{viii} —Zn1—Ti1 ^{xiii} | 113.811 (4) | Ti1 ^{vii} —O2—Ti1 ^v | 180.0 |
| Zn1 ^{xii} —Zn1—Ti1 ^{xiii} | 63.051 (4) | Ti1 ^{iv} —O2—Ti1 | 90.0 |
| Zn1 ^{xi} —Zn1—Ti1 ^{xiii} | 113.811 (4) | Ti1 ^{vi} —O2—Ti1 | 90.0 |
| Zn2 ^{viii} —Zn1—Ti1 ^{xiv} | 65.4310 (10) | Ti1 ⁱⁱ —O2—Ti1 | 180.0 |
| Zn2 ^{xi} —Zn1—Ti1 ^{xiv} | 168.380 (8) | Ti1 ^{vii} —O2—Ti1 | 90.0 |
| Zn2 ^{xii} —Zn1—Ti1 ^{xiv} | 65.4310 (10) | Ti1 ^v —O2—Ti1 | 90.0 |

Symmetry codes: (i) $-x+1/4, y, -z+1/4$; (ii) $-x+1/4, -y+1/4, z$; (iii) $x, -y+1/4, -z+1/4$; (iv) $-y+1/4, z, -x+1/4$; (v) $z, -x+1/4, -y+1/4$; (vi) y, z, x ; (vii) z, x, y ; (viii) $x, -y+3/4, -z+3/4$; (ix) $x, y-1/2, z-1/2$; (x) $x+1/4, y-1/4, -z+1/2$; (xi) $-x+3/4, y, -z+3/4$; (xii) $-x+3/4, -y+3/4, z$; (xiii) $y+1/4, -z+1/2, x-1/4$; (xiv) $-z+1/2, x-1/4, y+1/4$; (xv) $x-1/4, y+1/4, -z+1/2$; (xvi) $-x+1, y+1/4, z+1/4$; (xvii) $x+1/4, -y+1, z+1/4$; (xviii) $x+1/4, y+1/4, -z+1$; (xix) $x, y+1/2, z+1/2$; (xx) $-y+1/2, -z+1/2, -x+1$; (xxi) $y+1/2, z+1/2, x$; (xxii) $-z+1/2, -x+1, -y+1/2$; (xxiii) $z+1/2, x, y+1/2$; (xxiv) $-x+1, -y+1/2, -z+1/2$; (xxv) $y-1/4, -z, x-1/4$; (xxvi) $-z, x-1/4, y-1/4$; (xxvii) $x-1/4, y-1/4, -z$.

Ti₃Zn₃O_{1.27}

Crystal data

| | |
|---|---|
| Ti ₃ Zn ₃ O _{1.27} | $D_x = 6.244 \text{ Mg m}^{-3}$ |
| $M_r = 360.11$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Cubic, $Fd\bar{3}m$ | Cell parameters from 383 reflections |
| $a = 11.5286 (2) \text{ \AA}$ | $\theta = 3.1\text{--}36.0^\circ$ |
| $V = 1532.25 (8) \text{ \AA}^3$ | $\mu = 24.23 \text{ mm}^{-1}$ |
| $Z = 16$ | $T = 302 \text{ K}$ |
| $F(000) = 2658$ | Granule, black |
| | $0.05 \times 0.03 \times 0.03 \text{ mm}$ |

Data collection

| | |
|--|---|
| Radiation source: micro focus sealed tube | 243 reflections with $I > 2\sigma(I)$ |
| Detector resolution: $7.4074 \text{ pixels mm}^{-1}$ | $R_{\text{int}} = 0.030$ |
| ω, φ scans | $\theta_{\text{max}} = 39.2^\circ, \theta_{\text{min}} = 3.1^\circ$ |
| Absorption correction: multi-scan <i>SADABS2016/2</i> - Bruker AXS area detector scaling and absorption correction | $h = -20 \rightarrow 20$ |
| $T_{\text{min}} = 0.47, T_{\text{max}} = 0.58$ | $k = -20 \rightarrow 20$ |
| 23193 measured reflections | $l = -19 \rightarrow 20$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | $w = 1/[\sigma^2(F_o^2) + (0.0084P)^2 + 18.4301P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| Least-squares matrix: full | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| $R[F^2 > 2\sigma(F^2)] = 0.015$ | $\Delta\rho_{\text{max}} = 0.67 \text{ e \AA}^{-3}$ |
| $wR(F^2) = 0.031$ | $\Delta\rho_{\text{min}} = -0.49 \text{ e \AA}^{-3}$ |
| $S = 1.14$ | Extinction correction: <i>SHELXL2014/7</i> (Sheldrick 2014) |
| 252 reflections | Extinction coefficient: $0.00017 (4)$ |
| 25 parameters | |
| 1 restraint | |

Special details

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

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|-------------|-------------|-------------|----------------------------------|------------|
| Ti1a | 0.30635 (4) | 0.1250 | 0.1250 | 0.00557 (10) | 0.959 (2) |
| Ti1b | 0.3812 (9) | 0.1250 | 0.1250 | 0.007 (2)* | 0.041 |
| Zn1a | 0.29053 (5) | 0.29053 (5) | 0.29053 (5) | 0.00770 (14) | 0.982 (6) |
| Zn1b | 0.269 (4) | 0.269 (4) | 0.269 (4) | 0.017 (7)* | 0.018 |
| Zn2 | 0.5000 | 0.5000 | 0.5000 | 0.00963 (12) | |
| O1a | 0.0000 | 0.0000 | 0.0000 | 0.0040 (6) | 0.853 (10) |
| O1b | 0.0422 (6) | 0.0422 (6) | 0.0422 (6) | 0.002 (3)* | 0.147 |
| O2 | 0.1250 | 0.1250 | 0.1250 | 0.011 (4) | 0.24 (2) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|--------------|--------------|--------------|---------------|---------------|---------------|
| Ti1a | 0.00670 (17) | 0.00501 (11) | 0.00501 (11) | 0.000 | 0.000 | 0.00001 (11) |
| Zn1a | 0.00770 (14) | 0.00770 (14) | 0.00770 (14) | -0.00056 (10) | -0.00056 (10) | -0.00056 (10) |
| Zn2 | 0.00963 (12) | 0.00963 (12) | 0.00963 (12) | -0.00190 (9) | -0.00190 (9) | -0.00190 (9) |
| O1a | 0.0040 (6) | 0.0040 (6) | 0.0040 (6) | -0.0006 (5) | -0.0006 (5) | -0.0006 (5) |
| O2 | 0.011 (4) | 0.011 (4) | 0.011 (4) | 0.000 | 0.000 | 0.000 |

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

| | | | |
|--------------------------|------------|---------------------------|-----------|
| Ti1a—Ti1b | 0.863 (10) | Zn1b—Ti1b ^{xv} | 2.68 (3) |
| Ti1a—O1b ⁱ | 1.764 (3) | Zn1b—Ti1b ^{xvi} | 2.68 (3) |
| Ti1a—O1b ⁱⁱ | 1.764 (3) | Zn2—Ti1b ^{xvii} | 2.455 (5) |
| Ti1a—O2 | 2.0907 (4) | Zn2—Ti1b ^{xviii} | 2.455 (6) |
| Ti1a—O1a ⁱ | 2.1390 (1) | Zn2—Ti1b ^{xix} | 2.455 (5) |
| Ti1a—O1a ⁱⁱ | 2.1390 (1) | Zn2—Ti1b ^{xx} | 2.455 (5) |
| Ti1a—Zn1b ⁱⁱⁱ | 2.39 (5) | Zn2—Ti1b ^{xxi} | 2.455 (5) |

| | | | |
|---------------------------|-------------|----------------------------|------------|
| Ti1a—Zn1b | 2.39 (5) | Zn2—Ti1b ^{xxii} | 2.455 (5) |
| Ti1a—Zn1a | 2.7050 (8) | Zn2—Zn1a ^{xxiii} | 2.5036 (3) |
| Ti1a—Zn1a ⁱⁱⁱ | 2.7050 (8) | Zn2—Zn1a ^{xiii} | 2.5036 (3) |
| Ti1a—Ti1a ^{iv} | 2.9567 (6) | Zn2—Zn1a ^{xxiv} | 2.5036 (3) |
| Ti1a—Ti1a ^v | 2.9567 (6) | Zn2—Zn1a ^{viii} | 2.5036 (3) |
| Ti1b—Zn1a ^{vi} | 2.296 (8) | Zn2—Zn1a ^{xxv} | 2.5036 (3) |
| Ti1b—Zn1a ^{vii} | 2.296 (8) | Zn2—Zn1a ^{xiv} | 2.5036 (3) |
| Ti1b—Zn1b ^{vi} | 2.346 (16) | O1a—O1b ^{xxvi} | 0.843 (12) |
| Ti1b—Zn1b ^{vii} | 2.346 (16) | O1a—O1b | 0.843 (12) |
| Ti1b—O1b ⁱ | 2.412 (8) | O1a—Ti1a ⁱⁱ | 2.1390 (1) |
| Ti1b—O1b ⁱⁱ | 2.412 (8) | O1a—Ti1a ^{xxvii} | 2.1390 (1) |
| Ti1b—Zn2 ^{viii} | 2.455 (5) | O1a—Ti1a ^{iv} | 2.1390 (1) |
| Ti1b—Zn2 ^{ix} | 2.455 (5) | O1a—Ti1a ^{xxviii} | 2.1390 (1) |
| Ti1b—O1a ⁱⁱ | 2.538 (6) | O1a—Ti1a ^v | 2.1390 (1) |
| Ti1b—O1a ⁱ | 2.538 (6) | O1a—Ti1a ^{xxix} | 2.1390 (1) |
| Ti1b—Zn1b ⁱⁱⁱ | 2.68 (3) | O1a—Ti1b ^{xxix} | 2.538 (6) |
| Zn1a—Ti1b ^x | 2.296 (8) | O1a—Ti1b ^v | 2.538 (6) |
| Zn1a—Ti1b ^{xi} | 2.296 (8) | O1a—Ti1b ⁱⁱ | 2.538 (6) |
| Zn1a—Ti1b ^{xii} | 2.296 (8) | O1a—Ti1b ^{xxviii} | 2.538 (6) |
| Zn1a—Zn2 ^{viii} | 2.5037 (3) | O1b—O2 | 1.653 (12) |
| Zn1a—Zn2 ^{xiii} | 2.5037 (3) | O1b—O1b ^{xxvi} | 1.69 (2) |
| Zn1a—Zn2 ^{xiv} | 2.5037 (3) | O1b—Ti1a ⁱⁱ | 1.764 (3) |
| Zn1a—Ti1a ^{xv} | 2.7050 (8) | O1b—Ti1a ^{iv} | 1.764 (3) |
| Zn1a—Ti1a ^{xvi} | 2.7050 (8) | O1b—Ti1a ^v | 1.764 (3) |
| Zn1a—Zn1a ^{viii} | 2.7542 (16) | O1b—Ti1b ⁱⁱ | 2.412 (8) |
| Zn1a—Zn1a ^{xiv} | 2.7542 (16) | O1b—Ti1b ^v | 2.412 (8) |
| Zn1a—Zn1a ^{xiii} | 2.7542 (16) | O1b—Ti1b ^{iv} | 2.412 (8) |
| Zn1b—Ti1b ^{xi} | 2.346 (16) | O2—O1b ⁱⁱⁱ | 1.653 (12) |
| Zn1b—Ti1b ^x | 2.346 (16) | O2—O1b ⁱ | 1.653 (12) |
| Zn1b—Ti1b ^{xii} | 2.346 (16) | O2—O1b ⁱⁱ | 1.653 (12) |
| Zn1b—Ti1a ^{xvi} | 2.39 (5) | O2—Ti1a ⁱⁱ | 2.0907 (4) |
| Zn1b—Ti1a ^{xv} | 2.39 (5) | O2—Ti1a ^{iv} | 2.0907 (4) |

| | | | |
|---|--------------|---|-------------|
| Zn1b—Zn2 ^{viii} | 2.68 (3) | O2—Ti1a ^{xvi} | 2.0907 (4) |
| Zn1b—Zn2 ^{xiv} | 2.68 (3) | O2—Ti1a ^v | 2.0907 (4) |
| Zn1b—Zn2 ^{xiii} | 2.68 (3) | O2—Ti1a ^{xv} | 2.0907 (4) |
| Ti1b—Ti1a—O1b ⁱ | 130.1 (4) | Ti1a—Zn1b—Ti1b ^{xv} | 90.8 (18) |
| Ti1b—Ti1a—O1b ⁱⁱ | 130.1 (4) | Zn2 ^{viii} —Zn1b—Ti1b ^{xv} | 127.17 (14) |
| O1b ⁱ —Ti1a—O1b ⁱⁱ | 99.8 (8) | Zn2 ^{xiv} —Zn1b—Ti1b ^{xv} | 54.52 (19) |
| Ti1b—Ti1a—O2 | 180.0 | Zn2 ^{xiii} —Zn1b—Ti1b ^{xv} | 127.17 (14) |
| O1b ⁱ —Ti1a—O2 | 49.9 (4) | Ti1b ^{xi} —Zn1b—Ti1b ^{xvi} | 166 (3) |
| O1b ⁱⁱ —Ti1a—O2 | 49.9 (4) | Ti1b ^x —Zn1b—Ti1b ^{xvi} | 69.6 (4) |
| Ti1b—Ti1a—O1a ⁱ | 107.680 (11) | Ti1b ^{xii} —Zn1b—Ti1b ^{xvi} | 69.6 (4) |
| O1b ⁱ —Ti1a—O1a ⁱ | 22.4 (4) | Ti1a ^{xvi} —Zn1b—Ti1b ^{xvi} | 18.4 (2) |
| O1b ⁱⁱ —Ti1a—O1a ⁱ | 122.2 (4) | Ti1a ^{xv} —Zn1b—Ti1b ^{xvi} | 90.8 (18) |
| O2—Ti1a—O1a ⁱ | 72.320 (11) | Ti1a—Zn1b—Ti1b ^{xvi} | 90.8 (18) |
| Ti1b—Ti1a—O1a ⁱⁱ | 107.680 (11) | Zn2 ^{viii} —Zn1b—Ti1b ^{xvi} | 127.17 (14) |
| O1b ⁱ —Ti1a—O1a ⁱⁱ | 122.2 (4) | Zn2 ^{xiv} —Zn1b—Ti1b ^{xvi} | 127.17 (14) |
| O1b ⁱⁱ —Ti1a—O1a ⁱⁱ | 22.4 (4) | Zn2 ^{xiii} —Zn1b—Ti1b ^{xvi} | 54.52 (19) |
| O2—Ti1a—O1a ⁱⁱ | 72.320 (11) | Ti1b ^{xv} —Zn1b—Ti1b ^{xvi} | 102.2 (17) |
| O1a ⁱ —Ti1a—O1a ⁱⁱ | 144.64 (2) | Ti1b ^{xi} —Zn1b—Ti1b | 69.6 (4) |
| Ti1b—Ti1a—Zn1b ⁱⁱⁱ | 100.3 (12) | Ti1b ^x —Zn1b—Ti1b | 69.6 (4) |
| O1b ⁱ —Ti1a—Zn1b ⁱⁱⁱ | 83.4 (8) | Ti1b ^{xii} —Zn1b—Ti1b | 166 (3) |
| O1b ⁱⁱ —Ti1a—Zn1b ⁱⁱⁱ | 83.4 (8) | Ti1a ^{xvi} —Zn1b—Ti1b | 90.8 (18) |
| O2—Ti1a—Zn1b ⁱⁱⁱ | 79.7 (12) | Ti1a ^{xv} —Zn1b—Ti1b | 90.8 (18) |
| O1a ⁱ —Ti1a—Zn1b ⁱⁱⁱ | 86.9 (4) | Ti1a—Zn1b—Ti1b | 18.4 (2) |
| O1a ⁱⁱ —Ti1a—Zn1b ⁱⁱⁱ | 86.9 (4) | Zn2 ^{viii} —Zn1b—Ti1b | 54.52 (19) |
| Ti1b—Ti1a—Zn1b | 100.3 (12) | Zn2 ^{xiv} —Zn1b—Ti1b | 127.17 (14) |
| O1b ⁱ —Ti1a—Zn1b | 83.4 (8) | Zn2 ^{xiii} —Zn1b—Ti1b | 127.17 (14) |
| O1b ⁱⁱ —Ti1a—Zn1b | 83.4 (8) | Ti1b ^{xv} —Zn1b—Ti1b | 102.2 (17) |
| O2—Ti1a—Zn1b | 79.7 (12) | Ti1b ^{xvi} —Zn1b—Ti1b | 102.2 (17) |
| O1a ⁱ —Ti1a—Zn1b | 86.9 (4) | Ti1b ^{xvii} —Zn2—Ti1b ^{xviii} | 180.0 |
| O1a ⁱⁱ —Ti1a—Zn1b | 86.9 (4) | Ti1b ^{xvii} —Zn2—Ti1b ^{xix} | 108.1 (2) |
| Zn1b ⁱⁱⁱ —Ti1a—Zn1b | 159 (2) | Ti1b ^{xviii} —Zn2—Ti1b ^{xix} | 71.9 (2) |

| | | | |
|---|--------------|--|-------------|
| Ti1b—Ti1a—Zn1a | 93.865 (16) | Ti1b ^{xvii} —Zn2—Ti1b ^{xx} | 71.9 (2) |
| O1b ⁱ —Ti1a—Zn1a | 87.51 (2) | Ti1b ^{xviii} —Zn2—Ti1b ^{xx} | 108.1 (2) |
| O1b ⁱⁱ —Ti1a—Zn1a | 87.51 (2) | Ti1b ^{xix} —Zn2—Ti1b ^{xx} | 180.0 |
| O2—Ti1a—Zn1a | 86.135 (16) | Ti1b ^{xvii} —Zn2—Ti1b ^{xxi} | 108.1 (2) |
| O1a ⁱ —Ti1a—Zn1a | 88.827 (5) | Ti1b ^{xviii} —Zn2—Ti1b ^{xxi} | 71.9 (2) |
| O1a ⁱⁱ —Ti1a—Zn1a | 88.827 (5) | Ti1b ^{xix} —Zn2—Ti1b ^{xxi} | 108.1 (2) |
| Zn1b ⁱⁱⁱ —Ti1a—Zn1a | 165.8 (12) | Ti1b ^{xx} —Zn2—Ti1b ^{xxi} | 71.9 (2) |
| Zn1b—Ti1a—Zn1a | 6.4 (12) | Ti1b ^{xvii} —Zn2—Ti1b ^{xxii} | 71.9 (2) |
| Ti1b—Ti1a—Zn1a ⁱⁱⁱ | 93.864 (16) | Ti1b ^{xviii} —Zn2—Ti1b ^{xxii} | 108.1 (2) |
| O1b ⁱ —Ti1a—Zn1a ⁱⁱⁱ | 87.51 (2) | Ti1b ^{xix} —Zn2—Ti1b ^{xxii} | 71.9 (2) |
| O1b ⁱⁱ —Ti1a—Zn1a ⁱⁱⁱ | 87.51 (2) | Ti1b ^{xx} —Zn2—Ti1b ^{xxii} | 108.1 (2) |
| O2—Ti1a—Zn1a ⁱⁱⁱ | 86.136 (16) | Ti1b ^{xxi} —Zn2—Ti1b ^{xxii} | 180.0 |
| O1a ⁱ —Ti1a—Zn1a ⁱⁱⁱ | 88.827 (5) | Ti1b ^{xvii} —Zn2—Zn1a ^{xxiii} | 71.40 (19) |
| O1a ⁱⁱ —Ti1a—Zn1a ⁱⁱⁱ | 88.827 (5) | Ti1b ^{xviii} —Zn2—Zn1a ^{xxiii} | 108.60 (19) |
| Zn1b ⁱⁱⁱ —Ti1a—Zn1a ⁱⁱⁱ | 6.4 (12) | Ti1b ^{xix} —Zn2—Zn1a ^{xxiii} | 124.85 (14) |
| Zn1b—Ti1a—Zn1a ⁱⁱⁱ | 165.8 (12) | Ti1b ^{xx} —Zn2—Zn1a ^{xxiii} | 55.15 (14) |
| Zn1a—Ti1a—Zn1a ⁱⁱⁱ | 172.27 (3) | Ti1b ^{xxi} —Zn2—Zn1a ^{xxiii} | 124.85 (14) |
| Ti1b—Ti1a—Ti1a ^{iv} | 135.0 | Ti1b ^{xxii} —Zn2—Zn1a ^{xxiii} | 55.15 (14) |
| O1b ⁱ —Ti1a—Ti1a ^{iv} | 33.08 (15) | Ti1b ^{xvii} —Zn2—Zn1a ^{xxiii} | 108.60 (19) |
| O1b ⁱⁱ —Ti1a—Ti1a ^{iv} | 85.8 (3) | Ti1b ^{xviii} —Zn2—Zn1a ^{xxiii} | 71.40 (19) |
| O2—Ti1a—Ti1a ^{iv} | 45.0 | Ti1b ^{xix} —Zn2—Zn1a ^{xxiii} | 55.15 (14) |
| O1a ⁱ —Ti1a—Ti1a ^{iv} | 46.280 (8) | Ti1b ^{xx} —Zn2—Zn1a ^{xxiii} | 124.85 (14) |
| O1a ⁱⁱ —Ti1a—Ti1a ^{iv} | 105.167 (9) | Ti1b ^{xxi} —Zn2—Zn1a ^{xxiii} | 55.15 (14) |
| Zn1b ⁱⁱⁱ —Ti1a—Ti1a ^{iv} | 51.8 (9) | Ti1b ^{xxii} —Zn2—Zn1a ^{xxiii} | 124.85 (14) |
| Zn1b—Ti1a—Ti1a ^{iv} | 111.4 (10) | Zn1a ^{xxiii} —Zn2—Zn1a ^{xxiii} | 180.0 |
| Zn1a—Ti1a—Ti1a ^{iv} | 116.821 (13) | Ti1b ^{xvii} —Zn2—Zn1a ^{xxiv} | 124.85 (14) |
| Zn1a ⁱⁱⁱ —Ti1a—Ti1a ^{iv} | 56.872 (12) | Ti1b ^{xviii} —Zn2—Zn1a ^{xxiv} | 55.15 (14) |
| Ti1b—Ti1a—Ti1a ^v | 135.0 | Ti1b ^{xix} —Zn2—Zn1a ^{xxiv} | 124.85 (14) |
| O1b ⁱ —Ti1a—Ti1a ^v | 85.8 (3) | Ti1b ^{xx} —Zn2—Zn1a ^{xxiv} | 55.15 (14) |
| O1b ⁱⁱ —Ti1a—Ti1a ^v | 33.08 (15) | Ti1b ^{xxi} —Zn2—Zn1a ^{xxiv} | 71.40 (19) |
| O2—Ti1a—Ti1a ^v | 45.0 | Ti1b ^{xxii} —Zn2—Zn1a ^{xxiv} | 108.60 (19) |
| O1a ⁱ —Ti1a—Ti1a ^v | 105.167 (9) | Zn1a ^{xxiii} —Zn2—Zn1a ^{xxiv} | 66.74 (3) |

| | | | |
|---|--------------|---|-------------|
| O1a ⁱⁱ —Ti1a—Ti1a ^v | 46.280 (8) | Zn1a ^{xiii} —Zn2—Zn1a ^{xxiv} | 113.26 (3) |
| Zn1b ⁱⁱⁱ —Ti1a—Ti1a ^v | 51.8 (9) | Ti1b ^{xvii} —Zn2—Zn1a ^{viii} | 55.15 (14) |
| Zn1b—Ti1a—Ti1a ^v | 111.4 (10) | Ti1b ^{xviii} —Zn2—Zn1a ^{viii} | 124.85 (14) |
| Zn1a—Ti1a—Ti1a ^v | 116.821 (13) | Ti1b ^{xix} —Zn2—Zn1a ^{viii} | 55.15 (14) |
| Zn1a ⁱⁱⁱ —Ti1a—Ti1a ^v | 56.872 (12) | Ti1b ^{xx} —Zn2—Zn1a ^{viii} | 124.85 (14) |
| Ti1a ^{iv} —Ti1a—Ti1a ^v | 60.0 | Ti1b ^{xxi} —Zn2—Zn1a ^{viii} | 108.60 (19) |
| Ti1a—Ti1b—Zn1a ^{vi} | 143.14 (15) | Ti1b ^{xxii} —Zn2—Zn1a ^{viii} | 71.40 (19) |
| Ti1a—Ti1b—Zn1a ^{vii} | 143.14 (15) | Zn1a ^{xxiii} —Zn2—Zn1a ^{viii} | 113.26 (3) |
| Zn1a ^{vi} —Ti1b—Zn1a ^{vii} | 73.7 (3) | Zn1a ^{xiii} —Zn2—Zn1a ^{viii} | 66.74 (3) |
| Ti1a—Ti1b—Zn1b ^{vi} | 132.7 (17) | Zn1a ^{xxiv} —Zn2—Zn1a ^{viii} | 180.0 |
| Zn1a ^{vi} —Ti1b—Zn1b ^{vi} | 10.4 (17) | Ti1b ^{xvii} —Zn2—Zn1a ^{xxv} | 124.85 (14) |
| Zn1a ^{vii} —Ti1b—Zn1b ^{vi} | 84.1 (18) | Ti1b ^{xviii} —Zn2—Zn1a ^{xxv} | 55.15 (14) |
| Ti1a—Ti1b—Zn1b ^{vii} | 132.7 (17) | Ti1b ^{xix} —Zn2—Zn1a ^{xxv} | 71.40 (19) |
| Zn1a ^{vi} —Ti1b—Zn1b ^{vii} | 84.1 (18) | Ti1b ^{xx} —Zn2—Zn1a ^{xxv} | 108.60 (19) |
| Zn1a ^{vii} —Ti1b—Zn1b ^{vii} | 10.4 (17) | Ti1b ^{xxi} —Zn2—Zn1a ^{xxv} | 124.85 (14) |
| Zn1b ^{vi} —Ti1b—Zn1b ^{vii} | 95 (3) | Ti1b ^{xxii} —Zn2—Zn1a ^{xxv} | 55.15 (14) |
| Ti1a—Ti1b—O1b ⁱ | 34.0 (3) | Zn1a ^{xxiii} —Zn2—Zn1a ^{xxv} | 66.74 (3) |
| Zn1a ^{vi} —Ti1b—O1b ⁱ | 177.2 (4) | Zn1a ^{xiii} —Zn2—Zn1a ^{xxv} | 113.26 (3) |
| Zn1a ^{vii} —Ti1b—O1b ⁱ | 109.1 (3) | Zn1a ^{xxiv} —Zn2—Zn1a ^{xxv} | 66.74 (3) |
| Zn1b ^{vi} —Ti1b—O1b ⁱ | 166.7 (17) | Zn1a ^{viii} —Zn2—Zn1a ^{xxv} | 113.26 (3) |
| Zn1b ^{vii} —Ti1b—O1b ⁱ | 98.7 (17) | Ti1b ^{xvii} —Zn2—Zn1a ^{xiv} | 55.15 (14) |
| Ti1a—Ti1b—O1b ⁱⁱ | 34.0 (3) | Ti1b ^{xviii} —Zn2—Zn1a ^{xiv} | 124.85 (14) |
| Zn1a ^{vi} —Ti1b—O1b ⁱⁱ | 109.1 (3) | Ti1b ^{xix} —Zn2—Zn1a ^{xiv} | 108.60 (19) |
| Zn1a ^{vii} —Ti1b—O1b ⁱⁱ | 177.2 (4) | Ti1b ^{xx} —Zn2—Zn1a ^{xiv} | 71.40 (19) |
| Zn1b ^{vi} —Ti1b—O1b ⁱⁱ | 98.7 (17) | Ti1b ^{xxi} —Zn2—Zn1a ^{xiv} | 55.15 (14) |
| Zn1b ^{vii} —Ti1b—O1b ⁱⁱ | 166.7 (17) | Ti1b ^{xxii} —Zn2—Zn1a ^{xiv} | 124.85 (14) |
| O1b ⁱ —Ti1b—O1b ⁱⁱ | 68.0 (6) | Zn1a ^{xxiii} —Zn2—Zn1a ^{xiv} | 113.26 (3) |
| Ti1a—Ti1b—Zn2 ^{viii} | 123.90 (19) | Zn1a ^{xiii} —Zn2—Zn1a ^{xiv} | 66.74 (3) |
| Zn1a ^{vi} —Ti1b—Zn2 ^{viii} | 63.5 (2) | Zn1a ^{xxiv} —Zn2—Zn1a ^{xiv} | 113.26 (3) |
| Zn1a ^{vii} —Ti1b—Zn2 ^{viii} | 63.5 (2) | Zn1a ^{viii} —Zn2—Zn1a ^{xiv} | 66.74 (3) |
| Zn1b ^{vi} —Ti1b—Zn2 ^{viii} | 67.8 (8) | Zn1a ^{xxv} —Zn2—Zn1a ^{xiv} | 180.0 |
| Zn1b ^{vii} —Ti1b—Zn2 ^{viii} | 67.8 (8) | O1b ^{xxvi} —O1a—O1b | 180 (2) |

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| O1b ⁱ —Ti1b—Zn2 ^{viii} | 117.54 (14) | O1b ^{xxvi} —O1a—Ti1a ⁱⁱ | 127.056 (11) |
| O1b ⁱⁱ —Ti1b—Zn2 ^{viii} | 117.54 (14) | O1b—O1a—Ti1a ⁱⁱ | 52.944 (11) |
| Ti1a—Ti1b—Zn2 ^{ix} | 123.90 (19) | O1b ^{xxvi} —O1a—Ti1a ^{xxvii} | 52.944 (11) |
| Zn1a ^{vi} —Ti1b—Zn2 ^{ix} | 63.5 (2) | O1b—O1a—Ti1a ^{xxvii} | 127.056 (11) |
| Zn1a ^{vii} —Ti1b—Zn2 ^{ix} | 63.5 (2) | Ti1a ⁱⁱ —O1a—Ti1a ^{xxvii} | 180.00 (2) |
| Zn1b ^{vi} —Ti1b—Zn2 ^{ix} | 67.8 (8) | O1b ^{xxvi} —O1a—Ti1a ^{iv} | 127.056 (11) |
| Zn1b ^{vii} —Ti1b—Zn2 ^{ix} | 67.8 (8) | O1b—O1a—Ti1a ^{iv} | 52.944 (11) |
| O1b ⁱ —Ti1b—Zn2 ^{ix} | 117.54 (14) | Ti1a ⁱⁱ —O1a—Ti1a ^{iv} | 87.439 (15) |
| O1b ⁱⁱ —Ti1b—Zn2 ^{ix} | 117.54 (14) | Ti1a ^{xxvii} —O1a—Ti1a ^{iv} | 92.561 (15) |
| Zn2 ^{viii} —Ti1b—Zn2 ^{ix} | 112.2 (4) | O1b ^{xxvi} —O1a—Ti1a ^{xxviii} | 52.944 (11) |
| Ti1a—Ti1b—O1a ⁱⁱ | 53.42 (18) | O1b—O1a—Ti1a ^{xxviii} | 127.056 (11) |
| Zn1a ^{vi} —Ti1b—O1a ⁱⁱ | 89.72 (4) | Ti1a ⁱⁱ —O1a—Ti1a ^{xxviii} | 92.561 (15) |
| Zn1a ^{vii} —Ti1b—O1a ⁱⁱ | 163.4 (3) | Ti1a ^{xxvii} —O1a—Ti1a ^{xxviii} | 87.439 (15) |
| Zn1b ^{vi} —Ti1b—O1a ⁱⁱ | 79.3 (17) | Ti1a ^{iv} —O1a—Ti1a ^{xxviii} | 180.00 (2) |
| Zn1b ^{vii} —Ti1b—O1a ⁱⁱ | 173.9 (18) | O1b ^{xxvi} —O1a—Ti1a ^v | 127.056 (11) |
| O1b ⁱ —Ti1b—O1a ⁱⁱ | 87.4 (4) | O1b—O1a—Ti1a ^v | 52.944 (11) |
| O1b ⁱⁱ —Ti1b—O1a ⁱⁱ | 19.4 (3) | Ti1a ⁱⁱ —O1a—Ti1a ^v | 87.439 (15) |
| Zn2 ^{viii} —Ti1b—O1a ⁱⁱ | 109.416 (16) | Ti1a ^{xxvii} —O1a—Ti1a ^v | 92.561 (15) |
| Zn2 ^{ix} —Ti1b—O1a ⁱⁱ | 109.416 (16) | Ti1a ^{iv} —O1a—Ti1a ^v | 87.439 (15) |
| Ti1a—Ti1b—O1a ⁱ | 53.42 (18) | Ti1a ^{xxviii} —O1a—Ti1a ^v | 92.561 (15) |
| Zn1a ^{vi} —Ti1b—O1a ⁱ | 163.4 (3) | O1b ^{xxvi} —O1a—Ti1a ^{xxix} | 52.944 (11) |
| Zn1a ^{vii} —Ti1b—O1a ⁱ | 89.72 (4) | O1b—O1a—Ti1a ^{xxix} | 127.056 (11) |
| Zn1b ^{vi} —Ti1b—O1a ⁱ | 173.9 (18) | Ti1a ⁱⁱ —O1a—Ti1a ^{xxix} | 92.561 (15) |
| Zn1b ^{vii} —Ti1b—O1a ⁱ | 79.3 (17) | Ti1a ^{xxvii} —O1a—Ti1a ^{xxix} | 87.439 (15) |
| O1b ⁱ —Ti1b—O1a ⁱ | 19.4 (3) | Ti1a ^{iv} —O1a—Ti1a ^{xxix} | 92.561 (15) |
| O1b ⁱⁱ —Ti1b—O1a ⁱ | 87.4 (4) | Ti1a ^{xxviii} —O1a—Ti1a ^{xxix} | 87.439 (15) |
| Zn2 ^{viii} —Ti1b—O1a ⁱ | 109.416 (16) | Ti1a ^v —O1a—Ti1a ^{xxix} | 180.00 (2) |
| Zn2 ^{ix} —Ti1b—O1a ⁱ | 109.416 (16) | O1b ^{xxvi} —O1a—Ti1b ^{xxix} | 71.85 (18) |
| O1a ⁱⁱ —Ti1b—O1a ⁱ | 106.8 (4) | O1b—O1a—Ti1b ^{xxix} | 108.15 (18) |
| Ti1a—Ti1b—Zn1b ⁱⁱⁱ | 61.2 (14) | Ti1a ⁱⁱ —O1a—Ti1b ^{xxix} | 78.97 (13) |
| Zn1a ^{vi} —Ti1b—Zn1b ⁱⁱⁱ | 112.6 (10) | Ti1a ^{xxvii} —O1a—Ti1b ^{xxix} | 101.03 (13) |
| Zn1a ^{vii} —Ti1b—Zn1b ⁱⁱⁱ | 112.6 (10) | Ti1a ^{iv} —O1a—Ti1b ^{xxix} | 78.97 (13) |

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| Zn1b ^{vi} —Ti1b—Zn1b ⁱⁱⁱ | 109.0 (2) | Ti1a ^{xxviii} —O1a—Ti1b ^{xxix} | 101.03 (13) |
| Zn1b ^{vii} —Ti1b—Zn1b ⁱⁱⁱ | 109.0 (2) | Ti1a ^v —O1a—Ti1b ^{xxix} | 161.10 (18) |
| O1b ⁱ —Ti1b—Zn1b ⁱⁱⁱ | 66.5 (11) | Ti1a ^{xxix} —O1a—Ti1b ^{xxix} | 18.90 (18) |
| O1b ⁱⁱ —Ti1b—Zn1b ⁱⁱⁱ | 66.5 (11) | O1b ^{xxvi} —O1a—Ti1b ^v | 108.15 (18) |
| Zn2 ^{viii} —Ti1b—Zn1b ⁱⁱⁱ | 174.8 (14) | O1b—O1a—Ti1b ^v | 71.85 (18) |
| Zn2 ^{ix} —Ti1b—Zn1b ⁱⁱⁱ | 62.7 (14) | Ti1a ⁱⁱ —O1a—Ti1b ^v | 101.03 (13) |
| O1a ⁱⁱ —Ti1b—Zn1b ⁱⁱⁱ | 73.3 (8) | Ti1a ^{xxvii} —O1a—Ti1b ^v | 78.97 (13) |
| O1a ⁱ —Ti1b—Zn1b ⁱⁱⁱ | 73.3 (8) | Ti1a ^{iv} —O1a—Ti1b ^v | 101.03 (13) |
| Ti1b ^x —Zn1a—Ti1b ^{xi} | 119.923 (15) | Ti1a ^{xxviii} —O1a—Ti1b ^v | 78.97 (13) |
| Ti1b ^x —Zn1a—Ti1b ^{xii} | 119.923 (15) | Ti1a ^v —O1a—Ti1b ^v | 18.90 (18) |
| Ti1b ^{xi} —Zn1a—Ti1b ^{xii} | 119.923 (15) | Ti1a ^{xxix} —O1a—Ti1b ^v | 161.10 (18) |
| Ti1b ^x —Zn1a—Zn2 ^{viii} | 61.36 (6) | Ti1b ^{xxix} —O1a—Ti1b ^v | 180.0 |
| Ti1b ^{xi} —Zn1a—Zn2 ^{viii} | 61.36 (6) | O1b ^{xxvi} —O1a—Ti1b ⁱⁱ | 108.15 (18) |
| Ti1b ^{xii} —Zn1a—Zn2 ^{viii} | 158.45 (16) | O1b—O1a—Ti1b ⁱⁱ | 71.85 (18) |
| Ti1b ^x —Zn1a—Zn2 ^{xiii} | 61.36 (6) | Ti1a ⁱⁱ —O1a—Ti1b ⁱⁱ | 18.90 (18) |
| Ti1b ^{xi} —Zn1a—Zn2 ^{xiii} | 158.45 (16) | Ti1a ^{xxvii} —O1a—Ti1b ⁱⁱ | 161.10 (18) |
| Ti1b ^{xii} —Zn1a—Zn2 ^{xiii} | 61.36 (6) | Ti1a ^{iv} —O1a—Ti1b ⁱⁱ | 101.03 (13) |
| Zn2 ^{viii} —Zn1a—Zn2 ^{xiii} | 108.98 (2) | Ti1a ^{xxviii} —O1a—Ti1b ⁱⁱ | 78.97 (13) |
| Ti1b ^x —Zn1a—Zn2 ^{xiv} | 158.45 (16) | Ti1a ^v —O1a—Ti1b ⁱⁱ | 101.03 (13) |
| Ti1b ^{xi} —Zn1a—Zn2 ^{xiv} | 61.36 (6) | Ti1a ^{xxix} —O1a—Ti1b ⁱⁱ | 78.97 (13) |
| Ti1b ^{xii} —Zn1a—Zn2 ^{xiv} | 61.36 (6) | Ti1b ^{xxix} —O1a—Ti1b ⁱⁱ | 69.24 (17) |
| Zn2 ^{viii} —Zn1a—Zn2 ^{xiv} | 108.98 (2) | Ti1b ^v —O1a—Ti1b ⁱⁱ | 110.76 (17) |
| Zn2 ^{xiii} —Zn1a—Zn2 ^{xiv} | 108.98 (2) | O1b ^{xxvi} —O1a—Ti1b ^{xxviii} | 71.85 (18) |
| Ti1b ^x —Zn1a—Ti1a ^{xv} | 130.72 (15) | O1b—O1a—Ti1b ^{xxviii} | 108.15 (18) |
| Ti1b ^{xi} —Zn1a—Ti1a ^{xv} | 72.91 (12) | Ti1a ⁱⁱ —O1a—Ti1b ^{xxviii} | 78.97 (13) |
| Ti1b ^{xii} —Zn1a—Ti1a ^{xv} | 72.91 (12) | Ti1a ^{xxvii} —O1a—Ti1b ^{xxviii} | 101.03 (13) |
| Zn2 ^{viii} —Zn1a—Ti1a ^{xv} | 124.151 (18) | Ti1a ^{iv} —O1a—Ti1b ^{xxviii} | 161.10 (18) |
| Zn2 ^{xiii} —Zn1a—Ti1a ^{xv} | 124.151 (18) | Ti1a ^{xxviii} —O1a—Ti1b ^{xxviii} | 18.90 (18) |
| Zn2 ^{xiv} —Zn1a—Ti1a ^{xv} | 70.831 (12) | Ti1a ^v —O1a—Ti1b ^{xxviii} | 78.97 (13) |
| Ti1b ^x —Zn1a—Ti1a ^{xvi} | 72.91 (12) | Ti1a ^{xxix} —O1a—Ti1b ^{xxviii} | 101.03 (13) |
| Ti1b ^{xi} —Zn1a—Ti1a ^{xvi} | 130.72 (15) | Ti1b ^{xxix} —O1a—Ti1b ^{xxviii} | 110.76 (17) |
| Ti1b ^{xii} —Zn1a—Ti1a ^{xvi} | 72.91 (12) | Ti1b ^v —O1a—Ti1b ^{xxviii} | 69.24 (17) |

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| Zn2 ^{viii} —Zn1a—Ti1a ^{xvi} | 124.151 (18) | Ti1b ⁱⁱ —O1a—Ti1b ^{xxviii} | 69.24 (17) |
| Zn2 ^{xiii} —Zn1a—Ti1a ^{xvi} | 70.831 (12) | O1a—O1b—O2 | 180.0 (17) |
| Zn2 ^{xiv} —Zn1a—Ti1a ^{xvi} | 124.151 (18) | O1a—O1b—O1b ^{xxvi} | 0.0 (11) |
| Ti1a ^{xv} —Zn1a—Ti1a ^{xvi} | 66.26 (2) | O2—O1b—O1b ^{xxvi} | 180.0 (6) |
| Ti1b ^x —Zn1a—Ti1a | 72.91 (12) | O1a—O1b—Ti1a ⁱⁱ | 104.6 (4) |
| Ti1b ^{xi} —Zn1a—Ti1a | 72.91 (12) | O2—O1b—Ti1a ⁱⁱ | 75.4 (4) |
| Ti1b ^{xii} —Zn1a—Ti1a | 130.72 (15) | O1b ^{xxvi} —O1b—Ti1a ⁱⁱ | 104.6 (4) |
| Zn2 ^{viii} —Zn1a—Ti1a | 70.830 (12) | O1a—O1b—Ti1a ^{iv} | 104.6 (4) |
| Zn2 ^{xiii} —Zn1a—Ti1a | 124.151 (18) | O2—O1b—Ti1a ^{iv} | 75.4 (4) |
| Zn2 ^{xiv} —Zn1a—Ti1a | 124.151 (18) | O1b ^{xxvi} —O1b—Ti1a ^{iv} | 104.6 (4) |
| Ti1a ^{xv} —Zn1a—Ti1a | 66.26 (2) | Ti1a ⁱⁱ —O1b—Ti1a ^{iv} | 113.8 (3) |
| Ti1a ^{xvi} —Zn1a—Ti1a | 66.26 (2) | O1a—O1b—Ti1a ^v | 104.6 (4) |
| Ti1b ^x —Zn1a—Zn1a ^{viii} | 105.42 (13) | O2—O1b—Ti1a ^v | 75.4 (4) |
| Ti1b ^{xi} —Zn1a—Zn1a ^{viii} | 105.42 (13) | O1b ^{xxvi} —O1b—Ti1a ^v | 104.6 (4) |
| Ti1b ^{xii} —Zn1a—Zn1a ^{viii} | 53.14 (15) | Ti1a ⁱⁱ —O1b—Ti1a ^v | 113.8 (3) |
| Zn2 ^{viii} —Zn1a—Zn1a ^{viii} | 105.30 (2) | Ti1a ^{iv} —O1b—Ti1a ^v | 113.8 (3) |
| Zn2 ^{xiii} —Zn1a—Zn1a ^{viii} | 56.630 (17) | O1a—O1b—Ti1b ⁱⁱ | 88.7 (3) |
| Zn2 ^{xiv} —Zn1a—Zn1a ^{viii} | 56.630 (17) | O2—O1b—Ti1b ⁱⁱ | 91.3 (3) |
| Ti1a ^{xv} —Zn1a—Zn1a ^{viii} | 116.822 (13) | O1b ^{xxvi} —O1b—Ti1b ⁱⁱ | 88.7 (3) |
| Ti1a ^{xvi} —Zn1a—Zn1a ^{viii} | 116.822 (13) | Ti1a ⁱⁱ —O1b—Ti1b ⁱⁱ | 15.88 (16) |
| Ti1a—Zn1a—Zn1a ^{viii} | 176.134 (16) | Ti1a ^{iv} —O1b—Ti1b ⁱⁱ | 119.29 (13) |
| Ti1b ^x —Zn1a—Zn1a ^{xiv} | 53.14 (15) | Ti1a ^v —O1b—Ti1b ⁱⁱ | 119.29 (13) |
| Ti1b ^{xi} —Zn1a—Zn1a ^{xiv} | 105.42 (13) | O1a—O1b—Ti1b ^v | 88.7 (3) |
| Ti1b ^{xii} —Zn1a—Zn1a ^{xiv} | 105.42 (13) | O2—O1b—Ti1b ^v | 91.3 (3) |
| Zn2 ^{viii} —Zn1a—Zn1a ^{xiv} | 56.630 (17) | O1b ^{xxvi} —O1b—Ti1b ^v | 88.7 (3) |
| Zn2 ^{xiii} —Zn1a—Zn1a ^{xiv} | 56.630 (17) | Ti1a ⁱⁱ —O1b—Ti1b ^v | 119.29 (13) |
| Zn2 ^{xiv} —Zn1a—Zn1a ^{xiv} | 105.30 (2) | Ti1a ^{iv} —O1b—Ti1b ^v | 119.29 (13) |
| Ti1a ^{xv} —Zn1a—Zn1a ^{xiv} | 176.135 (16) | Ti1a ^v —O1b—Ti1b ^v | 15.88 (16) |
| Ti1a ^{xvi} —Zn1a—Zn1a ^{xiv} | 116.822 (13) | Ti1b ⁱⁱ —O1b—Ti1b ^v | 119.95 (2) |
| Ti1a—Zn1a—Zn1a ^{xiv} | 116.821 (13) | O1a—O1b—Ti1b ^{iv} | 88.7 (3) |
| Zn1a ^{viii} —Zn1a—Zn1a ^{xiv} | 60.0 | O2—O1b—Ti1b ^{iv} | 91.3 (3) |
| Ti1b ^x —Zn1a—Zn1a ^{xiii} | 105.42 (13) | O1b ^{xxvi} —O1b—Ti1b ^{iv} | 88.7 (3) |

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| Ti1b ^{xi} —Zn1a—Zn1a ^{xiii} | 53.14 (15) | Ti1a ⁱⁱ —O1b—Ti1b ^{iv} | 119.29 (13) |
| Ti1b ^{xii} —Zn1a—Zn1a ^{xiii} | 105.42 (13) | Ti1a ^{iv} —O1b—Ti1b ^{iv} | 15.88 (16) |
| Zn2 ^{viii} —Zn1a—Zn1a ^{xiii} | 56.630 (17) | Ti1a ^v —O1b—Ti1b ^{iv} | 119.29 (13) |
| Zn2 ^{xiii} —Zn1a—Zn1a ^{xiii} | 105.30 (2) | Ti1b ⁱⁱ —O1b—Ti1b ^{iv} | 119.95 (2) |
| Zn2 ^{xiv} —Zn1a—Zn1a ^{xiii} | 56.630 (17) | Ti1b ^v —O1b—Ti1b ^{iv} | 119.95 (2) |
| Ti1a ^{xv} —Zn1a—Zn1a ^{xiii} | 116.822 (13) | O1b—O2—O1b ⁱⁱⁱ | 109.5 |
| Ti1a ^{xvi} —Zn1a—Zn1a ^{xiii} | 176.135 (16) | O1b—O2—O1b ⁱ | 109.5 |
| Ti1a—Zn1a—Zn1a ^{xiii} | 116.821 (13) | O1b ⁱⁱⁱ —O2—O1b ⁱ | 109.5 |
| Zn1a ^{viii} —Zn1a—Zn1a ^{xiii} | 59.999 (1) | O1b—O2—O1b ⁱⁱ | 109.471 (1) |
| Zn1a ^{xiv} —Zn1a—Zn1a ^{xiii} | 60.0 | O1b ⁱⁱⁱ —O2—O1b ⁱⁱ | 109.471 (1) |
| Ti1b ^{xi} —Zn1b—Ti1b ^x | 115.8 (12) | O1b ⁱ —O2—O1b ⁱⁱ | 109.471 (1) |
| Ti1b ^{xi} —Zn1b—Ti1b ^{xii} | 115.8 (12) | O1b—O2—Ti1a ⁱⁱ | 54.7 |
| Ti1b ^x —Zn1b—Ti1b ^{xii} | 115.8 (12) | O1b ⁱⁱⁱ —O2—Ti1a ⁱⁱ | 54.7 |
| Ti1b ^{xi} —Zn1b—Ti1a ^{xvi} | 148 (3) | O1b ⁱ —O2—Ti1a ⁱⁱ | 125.3 |
| Ti1b ^x —Zn1b—Ti1a ^{xvi} | 78.3 (7) | O1b ⁱⁱ —O2—Ti1a ⁱⁱ | 125.3 |
| Ti1b ^{xii} —Zn1b—Ti1a ^{xvi} | 78.3 (7) | O1b—O2—Ti1a ^{iv} | 54.7 |
| Ti1b ^{xi} —Zn1b—Ti1a ^{xv} | 78.3 (7) | O1b ⁱⁱⁱ —O2—Ti1a ^{iv} | 125.3 |
| Ti1b ^x —Zn1b—Ti1a ^{xv} | 148 (3) | O1b ⁱ —O2—Ti1a ^{iv} | 54.7 |
| Ti1b ^{xii} —Zn1b—Ti1a ^{xv} | 78.3 (7) | O1b ⁱⁱ —O2—Ti1a ^{iv} | 125.3 |
| Ti1a ^{xvi} —Zn1b—Ti1a ^{xv} | 76.4 (19) | Ti1a ⁱⁱ —O2—Ti1a ^{iv} | 90.0 |
| Ti1b ^{xi} —Zn1b—Ti1a | 78.3 (7) | O1b—O2—Ti1a ^{xvi} | 125.3 |
| Ti1b ^x —Zn1b—Ti1a | 78.3 (7) | O1b ⁱⁱⁱ —O2—Ti1a ^{xvi} | 54.7 |
| Ti1b ^{xii} —Zn1b—Ti1a | 148 (3) | O1b ⁱ —O2—Ti1a ^{xvi} | 54.7 |
| Ti1a ^{xvi} —Zn1b—Ti1a | 76.4 (19) | O1b ⁱⁱ —O2—Ti1a ^{xvi} | 125.3 |
| Ti1a ^{xv} —Zn1b—Ti1a | 76.4 (19) | Ti1a ⁱⁱ —O2—Ti1a ^{xvi} | 90.0 |
| Ti1b ^{xi} —Zn1b—Zn2 ^{viii} | 58.1 (7) | Ti1a ^{iv} —O2—Ti1a ^{xvi} | 90.0 |
| Ti1b ^x —Zn1b—Zn2 ^{viii} | 58.1 (7) | O1b—O2—Ti1a ^v | 54.7 |
| Ti1b ^{xii} —Zn1b—Zn2 ^{viii} | 139 (3) | O1b ⁱⁱⁱ —O2—Ti1a ^v | 125.3 |
| Ti1a ^{xvi} —Zn1b—Zn2 ^{viii} | 130.4 (7) | O1b ⁱ —O2—Ti1a ^v | 125.3 |
| Ti1a ^{xv} —Zn1b—Zn2 ^{viii} | 130.4 (7) | O1b ⁱⁱ —O2—Ti1a ^v | 54.7 |
| Ti1a—Zn1b—Zn2 ^{viii} | 72.96 (12) | Ti1a ⁱⁱ —O2—Ti1a ^v | 90.0 |
| Ti1b ^{xi} —Zn1b—Zn2 ^{xiv} | 58.1 (7) | Ti1a ^{iv} —O2—Ti1a ^v | 90.0 |

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| Ti1b ^x —Zn1b—Zn2 ^{xiv} | 139 (3) | Ti1a ^{xvi} —O2—Ti1a ^v | 180.0 |
| Ti1b ^{xii} —Zn1b—Zn2 ^{xiv} | 58.1 (7) | O1b—O2—Ti1a ^{xv} | 125.3 |
| Ti1a ^{xvi} —Zn1b—Zn2 ^{xiv} | 130.4 (7) | O1b ⁱⁱⁱ —O2—Ti1a ^{xv} | 54.7 |
| Ti1a ^{xv} —Zn1b—Zn2 ^{xiv} | 72.96 (12) | O1b ⁱ —O2—Ti1a ^{xv} | 125.3 |
| Ti1a—Zn1b—Zn2 ^{xiv} | 130.4 (7) | O1b ⁱⁱ —O2—Ti1a ^{xv} | 54.7 |
| Zn2 ^{viii} —Zn1b—Zn2 ^{xiv} | 99.1 (17) | Ti1a ⁱⁱ —O2—Ti1a ^{xv} | 90.0 |
| Ti1b ^{xi} —Zn1b—Zn2 ^{xiii} | 139 (3) | Ti1a ^{iv} —O2—Ti1a ^{xv} | 180.0 |
| Ti1b ^x —Zn1b—Zn2 ^{xiii} | 58.1 (7) | Ti1a ^{xvi} —O2—Ti1a ^{xv} | 90.0 |
| Ti1b ^{xii} —Zn1b—Zn2 ^{xiii} | 58.1 (7) | Ti1a ^v —O2—Ti1a ^{xv} | 90.0 |
| Ti1a ^{xvi} —Zn1b—Zn2 ^{xiii} | 72.96 (12) | O1b—O2—Ti1a | 125.3 |
| Ti1a ^{xv} —Zn1b—Zn2 ^{xiii} | 130.4 (7) | O1b ⁱⁱⁱ —O2—Ti1a | 125.3 |
| Ti1a—Zn1b—Zn2 ^{xiii} | 130.4 (7) | O1b ⁱ —O2—Ti1a | 54.7 |
| Zn2 ^{viii} —Zn1b—Zn2 ^{xiii} | 99.1 (17) | O1b ⁱⁱ —O2—Ti1a | 54.7 |
| Zn2 ^{xiv} —Zn1b—Zn2 ^{xiii} | 99.1 (17) | Ti1a ⁱⁱ —O2—Ti1a | 180.0 |
| Ti1b ^{xi} —Zn1b—Ti1b ^{xv} | 69.6 (4) | Ti1a ^{iv} —O2—Ti1a | 90.0 |
| Ti1b ^x —Zn1b—Ti1b ^{xv} | 166 (3) | Ti1a ^{xvi} —O2—Ti1a | 90.0 |
| Ti1b ^{xii} —Zn1b—Ti1b ^{xv} | 69.6 (4) | Ti1a ^v —O2—Ti1a | 90.0 |
| Ti1a ^{xvi} —Zn1b—Ti1b ^{xv} | 90.8 (18) | Ti1a ^{xv} —O2—Ti1a | 90.0 |
| Ti1a ^{xv} —Zn1b—Ti1b ^{xv} | 18.4 (2) | | |

Symmetry codes: (i) $-x+1/4, y, -z+1/4$; (ii) $-x+1/4, -y+1/4, z$; (iii) $x, -y+1/4, -z+1/4$; (iv) $z, -x+1/4, -y+1/4$; (v) $-y+1/4, z, -x+1/4$; (vi) $x+1/4, -y+1/2, z-1/4$; (vii) $x+1/4, y-1/4, -z+1/2$; (viii) $x, -y+3/4, -z+3/4$; (ix) $x, y-1/2, z-1/2$; (x) $-z+1/2, x-1/4, y+1/4$; (xi) $y+1/4, -z+1/2, x-1/4$; (xii) $x-1/4, y+1/4, -z+1/2$; (xiii) $-x+3/4, -y+3/4, z$; (xiv) $-x+3/4, y, -z+3/4$; (xv) z, x, y ; (xvi) y, z, x ; (xvii) $-y+1/2, -z+1/2, -x+1$; (xviii) $y+1/2, z+1/2, x$; (xix) $-z+1/2, -x+1, -y+1/2$; (xx) $z+1/2, x, y+1/2$; (xxi) $-x+1, -y+1/2, -z+1/2$; (xxii) $x, y+1/2, z+1/2$; (xxiii) $x+1/4, y+1/4, -z+1$; (xxiv) $-x+1, y+1/4, z+1/4$; (xxv) $x+1/4, -y+1, z+1/4$; (xxvi) $-x, -y, -z$; (xxvii) $x-1/4, y-1/4, -z$; (xxviii) $-z, x-1/4, y-1/4$; (xxix) $y-1/4, -z, x-1/4$.