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Supporting information for article:

The crystal structure of the first synthetic copper(II) tellurite arsenate, $Cu^{II}5(Te^{IV}O3)2(As^{V}O4)2$

Owen Peter Missen, Matthias Weil, Stuart James Mills and Eugen Libowitzky

The crystal structure of the first synthetic copper(II) tellurite arsenate, $Cu^{II}_5(Te^{IV}O_3)_2(As^{V}O_4)_2$

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018*/3 (Sheldrick, 2015b); molecular graphics: *CrystalMaker* (Palmer, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

pentacopper(II) bis-oxotellurate(IV) bis-oxoarsenate(V)

Crystal data

$As_2Cu_5O_{14}Te_2$
M_r = 946.74
Triclinic, $P\overline{1}$
a = 4.9929 (8) Å
b = 7.8796 (12) Å
c = 8.1428 (12) Å
α = 77.333 (3)°
β = 79.233 (3)°
γ = 71.862 (3)°
V = 294.59 (8) Å^3
Z = 1
$F(000)$ = 427
D_x = 5.337 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4198 reflections
θ = 2.5–30.0°
μ = 19.39 mm^{-1}
T = 100 K
Fragment, dark green
0.08 × 0.07 × 0.06 mm

Data collection

Bruker APEX-II CCD diffractometer
ω– and φ–scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.449, T_{max} = 0.747
7545 measured reflections
2581 independent reflections
2347 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 35.0°, θ_{min} = 2.6°
h = −8→8
k = −12→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.062
S = 1.10
2581 reflections
106 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.025P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.26 e Å^{-3}
$\Delta\rho_{min}$ = −2.92 e Å^{-}

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 (Å²) for $Cu^{II}_5(Te^{IV}O_3)_2(As^{V}O_4)_2$

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	1.23462 (8)	0.99911 (5)	0.11680 (5)	0.00313 (7)
Cu2	0.89747 (8)	0.82328 (5)	0.49911 (5)	0.00314 (7)
Cu3	0.500000	0.500000	0.500000	0.00292 (9)
Te1	0.92519 (4)	0.66465 (2)	0.19225 (2)	0.00232 (5)
As1	0.37274 (6)	0.76681 (4)	0.74042 (4)	0.00213 (6)
O1	0.6356 (5)	0.8501 (3)	0.0918 (3)	0.0050 (4)
O2	1.0984 (5)	0.8112 (3)	0.2695 (3)	0.0043 (4)
O3	0.7491 (5)	0.6495 (3)	0.4229 (3)	0.0047 (4)
O4	0.2158 (5)	0.8841 (3)	0.5684 (3)	0.0044 (4)
O5	0.6879 (5)	0.8115 (3)	0.7257 (3)	0.0052 (4)
O6	0.1514 (5)	0.8242 (3)	0.9175 (3)	0.0037 (4)
O7	0.4350 (5)	0.5424 (3)	0.7362 (3)	0.0047 (4)

Atomic displacement parameters (Å²) for $Cu^{II}_5(Te^{IV}O_3)_2(As^{V}O_4)_2$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.00209 (15)	0.00302 (15)	0.00338 (16)	−0.00055 (12)	0.00034 (11)	0.00048 (12)
Cu2	0.00355 (15)	0.00413 (15)	0.00223 (16)	−0.00218 (12)	0.00071 (12)	−0.00086 (12)
Cu3	0.0036 (2)	0.0029 (2)	0.0026 (2)	−0.00185 (16)	0.00071 (16)	−0.00065 (16)
Te1	0.00240 (8)	0.00206 (8)	0.00223 (9)	−0.00041 (6)	−0.00012 (6)	−0.00028 (6)
As1	0.00195 (12)	0.00217 (12)	0.00213 (13)	−0.00060 (9)	0.00014 (9)	−0.00038 (9)
O1	0.0031 (9)	0.0053 (9)	0.0052 (10)	−0.0011 (7)	−0.0003 (7)	0.0016 (7)
O2	0.0056 (9)	0.0054 (9)	0.0026 (9)	−0.0029 (7)	0.0006 (7)	−0.0010 (7)
O3	0.0060 (9)	0.0063 (9)	0.0030 (9)	−0.0040 (8)	0.0010 (7)	−0.0012 (7)
O4	0.0046 (9)	0.0047 (9)	0.0038 (9)	−0.0010 (7)	−0.0024 (7)	0.0008 (7)
O5	0.0042 (9)	0.0090 (10)	0.0040 (9)	−0.0043 (8)	0.0012 (7)	−0.0021 (7)
O6	0.0045 (9)	0.0043 (9)	0.0022 (9)	−0.0016 (7)	0.0003 (7)	−0.0001 (7)
O7	0.0071 (10)	0.0021 (8)	0.0040 (9)	−0.0009 (7)	0.0005 (7)	−0.0003 (7)

Geometric parameters (Å, º) for $Cu^{II}_5(Te^{IV}O_3)_2(As^{V}O_4)_2$

Cu1—O2	1.925 (2)	Cu3—O7	1.975 (2)
Cu1—O1^{i}	1.975 (2)	Cu3—O4^{vi}	3.042 (2)
Cu1—O1^{ii}	1.979 (2)	Cu3—O4	3.042 (2)
Cu1—O6^{iii}	2.023 (2)	Te1—O1	1.870 (2)
Cu1—O5^{iv}	2.325 (2)	Te1—O2	1.902 (2)
Cu1—O6^{v}	2.509 (2)	Te1—O3	1.914 (2)
Cu2—O5	1.942 (2)	Te1—O6^{v}	2.563 (2)
Cu2—O2	1.957 (2)	Te1—O7^{vi}	2.693 (2)
Cu2—O3	1.996 (2)	Te1—O7^{vii}	3.200 (2)
Cu2—O4^{ii}	2.001 (2)	As1—O4	1.680 (2)
Cu2—O4^{iii}	2.165 (2)	As1—O5	1.694 (2)
Cu3—O3	1.904 (2)	As1—O6	1.698 (2)
Cu3—O3^{vi}	1.904 (2)	As1—O7	1.704 (2)
Cu3—O7^{vi}	1.975 (2)		
O2—Cu1—O1^{i}	162.28 (9)	Cu2—O3—Cu3^{ii}	62.27 (6)
O2—Cu1—O1^{ii}	94.72 (9)	Cu2^{vii}—O3—Cu3^{ii}	60.97 (4)
O1^{i}—Cu1—O1^{ii}	83.00 (10)	Cu3—O3—Cu1^{viii}	93.38 (8)
O2—Cu1—O6^{iii}	96.58 (9)	Te1—O3—Cu1^{viii}	68.91 (7)
O1^{i}—Cu1—O6^{iii}	83.76 (9)	Cu2—O3—Cu1^{viii}	98.48 (8)
O1^{ii}—Cu1—O6^{iii}	166.08 (9)	Cu2^{vii}—O3—Cu1^{viii}	139.34 (6)
O2—Cu1—O5^{iv}	108.98 (8)	Cu3^{ii}—O3—Cu1^{viii}	141.33 (6)
O1^{i}—Cu1—O5^{iv}	88.74 (8)	Cu3—O3—Cu2^{viii}	54.11 (6)
O1^{ii}—Cu1—O5^{iv}	94.77 (8)	Te1—O3—Cu2^{viii}	116.93 (9)
O6^{iii}—Cu1—O5^{iv}	89.22 (8)	Cu2—O3—Cu2^{viii}	107.60 (8)
O2—Cu1—O6^{v}	77.44 (8)	Cu2^{vii}—O3—Cu2^{viii}	119.99 (5)
O1^{i}—Cu1—O6^{v}	84.87 (8)	Cu3^{ii}—O3—Cu2^{viii}	161.35 (6)
O1^{ii}—Cu1—O6^{v}	86.54 (8)	Cu1^{viii}—O3—Cu2^{viii}	51.87 (3)
O6^{iii}—Cu1—O6^{v}	88.00 (8)	Cu3—O3—Cu1	164.22 (9)
O5^{iv}—Cu1—O6^{v}	173.28 (8)	Te1—O3—Cu1	47.95 (5)
O5—Cu2—O2	173.75 (8)	Cu2—O3—Cu1	52.37 (5)
O5—Cu2—O3	96.68 (9)	Cu2^{vii}—O3—Cu1	117.05 (6)
O2—Cu2—O3	77.29 (9)	Cu3^{ii}—O3—Cu1	67.20 (3)
O5—Cu2—O4^{ii}	93.67 (9)	Cu1^{viii}—O3—Cu1	74.54 (4)
O2—Cu2—O4^{ii}	90.90 (9)	Cu2^{viii}—O3—Cu1	120.63 (6)
O3—Cu2—O4^{ii}	150.30 (10)	As1—O4—Cu2^{viii}	122.06 (12)
O5—Cu2—O4^{iii}	97.02 (9)	As1—O4—Cu2^{iii}	123.88 (11)
O2—Cu2—O4^{iii}	88.14 (9)	Cu2^{viii}—O4—Cu2^{iii}	102.76 (9)
O3—Cu2—O4^{iii}	128.57 (9)	As1—O4—Cu3	73.46 (8)
O4^{ii}—Cu2—O4^{iii}	77.24 (10)	Cu2^{viii}—O4—Cu3	78.21 (7)
O3—Cu3—O3^{vi}	180.0	Cu2^{iii}—O4—Cu3	154.16 (10)
O3—Cu3—O7^{vi}	85.85 (9)	As1—O4—Cu1^{iii}	74.77 (8)
O3^{vi}—Cu3—O7^{vi}	94.15 (9)	Cu2^{viii}—O4—Cu1^{iii}	84.03 (7)
O3—Cu3—O7	94.15 (9)	Cu2^{iii}—O4—Cu1^{iii}	78.63 (7)
O3^{vi}—Cu3—O7	85.85 (9)	Cu3—O4—Cu1^{iii}	126.78 (7)
O7^{vi}—Cu3—O7	180.0	As1—O4—Cu2	68.48 (7)
O3—Cu3—O4^{vi}	111.53 (8)	Cu2^{viii}—O4—Cu2	143.35 (10)
O3^{vi}—Cu3—O4^{vi}	68.47 (8)	Cu2^{iii}—O4—Cu2	95.80 (7)
O7^{vi}—Cu3—O4^{vi}	61.52 (8)	Cu3—O4—Cu2	71.66 (5)
O7—Cu3—O4^{vi}	118.48 (8)	Cu1^{iii}—O4—Cu2	130.97 (7)
O3—Cu3—O4	68.47 (8)	As1—O4—Cu1^{viii}	150.07 (11)
O3^{vi}—Cu3—O4	111.53 (8)	Cu2^{viii}—O4—Cu1^{viii}	70.55 (6)

O7^{vi}—Cu3—O4	118.48 (8)	Cu2^{iii}—O4—Cu1^{viii}	72.15 (6)
O7—Cu3—O4	61.52 (8)	Cu3—O4—Cu1^{viii}	84.23 (5)
O4^{vi}—Cu3—O4	180.00 (9)	Cu1^{iii}—O4—Cu1^{viii}	135.15 (7)
O1—Te1—O2	98.28 (10)	Cu2—O4—Cu1^{viii}	85.89 (5)
O1—Te1—O3	98.60 (10)	As1—O5—Cu2	114.22 (12)
O2—Te1—O3	80.60 (9)	As1—O5—Cu1^{iv}	123.65 (12)
O1—Te1—O6^{v}	72.13 (8)	Cu2—O5—Cu1^{iv}	113.30 (9)
O2—Te1—O6^{v}	76.44 (8)	As1—O5—Cu3	51.17 (6)
O3—Te1—O6^{v}	153.50 (8)	Cu2—O5—Cu3	71.98 (6)
O1—Te1—O7^{vi}	87.12 (8)	Cu1^{iv}—O5—Cu3	174.51 (9)
O2—Te1—O7^{vi}	148.15 (8)	As1—O5—Cu2^{iii}	62.76 (7)
O3—Te1—O7^{vi}	67.55 (8)	Cu2—O5—Cu2^{iii}	83.14 (8)
O6^{v}—Te1—O7^{vi}	134.38 (7)	Cu1^{iv}—O5—Cu2^{iii}	95.28 (7)
O1—Te1—O7^{vii}	155.80 (8)	Cu3—O5—Cu2^{iii}	83.72 (5)
O2—Te1—O7^{vii}	67.34 (8)	As1—O5—Cu1^{ix}	74.37 (8)
O3—Te1—O7^{vii}	98.03 (8)	Cu2—O5—Cu1^{ix}	156.20 (10)
O6^{v}—Te1—O7^{vii}	85.24 (6)	Cu1^{iv}—O5—Cu1^{ix}	50.42 (5)
O7^{vi}—Te1—O7^{vii}	115.55 (7)	Cu3—O5—Cu1^{ix}	124.11 (6)
O4—As1—O5	108.42 (11)	Cu2^{iii}—O5—Cu1^{ix}	81.71 (5)
O4—As1—O6	109.10 (11)	As1—O5—Cu2^{iv}	142.03 (11)
O5—As1—O6	112.56 (10)	Cu2—O5—Cu2^{iv}	54.16 (5)
O4—As1—O7	107.25 (11)	Cu1^{iv}—O5—Cu2^{iv}	60.04 (5)
O5—As1—O7	108.90 (11)	Cu3—O5—Cu2^{iv}	124.85 (6)
O6—As1—O7	110.45 (10)	Cu2^{iii}—O5—Cu2^{iv}	79.42 (5)
Te1—O1—Cu1^{i}	114.83 (11)	Cu1^{ix}—O5—Cu2^{iv}	104.82 (5)
Te1—O1—Cu1^{viii}	147.17 (13)	As1—O5—Cu3^{ii}	125.49 (10)
Cu1^{i}—O1—Cu1^{viii}	97.00 (10)	Cu2—O5—Cu3^{ii}	45.37 (5)
Te1—O1—Cu1	67.20 (6)	Cu1^{iv}—O5—Cu3^{ii}	109.18 (7)
Cu1^{i}—O1—Cu1	64.76 (6)	Cu3—O5—Cu3^{ii}	75.46 (4)
Cu1^{viii}—O1—Cu1	124.88 (9)	Cu2^{iii}—O5—Cu3^{ii}	128.09 (6)
Te1—O1—Cu2	52.76 (5)	Cu1^{ix}—O5—Cu3^{ii}	148.33 (6)
Cu1^{i}—O1—Cu2	119.86 (8)	Cu2^{iv}—O5—Cu3^{ii}	75.02 (4)
Cu1^{viii}—O1—Cu2	105.13 (8)	As1—O6—Cu1^{iii}	116.95 (12)
Cu1—O1—Cu2	56.59 (3)	As1—O6—Cu1^{ix}	125.30 (10)
Te1—O1—Cu3	56.32 (6)	Cu1^{iii}—O6—Cu1^{ix}	91.99 (8)
Cu1^{i}—O1—Cu3	171.00 (10)	As1—O6—Cu1^{iv}	72.21 (7)
Cu1^{viii}—O1—Cu3	92.00 (7)	Cu1^{iii}—O6—Cu1^{iv}	119.12 (8)
Cu1—O1—Cu3	110.07 (6)	Cu1^{ix}—O6—Cu1^{iv}	53.09 (4)
Cu2—O1—Cu3	57.44 (3)	As1—O6—Cu2^{viii}	55.89 (6)
Te1—O2—Cu1	121.75 (12)	Cu1^{iii}—O6—Cu2^{viii}	66.61 (6)
Te1—O2—Cu2	101.70 (10)	Cu1^{ix}—O6—Cu2^{viii}	149.05 (8)
Cu1—O2—Cu2	126.80 (11)	Cu1^{iv}—O6—Cu2^{viii}	116.91 (6)
Te1—O2—Cu3^{ii}	97.89 (8)	As1—O6—Cu2^{iii}	61.13 (7)
Cu1—O2—Cu3^{ii}	121.31 (9)	Cu1^{iii}—O6—Cu2^{iii}	63.15 (6)
Cu2—O2—Cu3^{ii}	76.16 (7)	Cu1^{ix}—O6—Cu2^{iii}	101.24 (6)
Te1—O2—Cu1^{i}	62.66 (6)	Cu1^{iv}—O6—Cu2^{iii}	75.92 (4)
Cu1—O2—Cu1^{i}	63.71 (6)	Cu2^{viii}—O6—Cu2^{iii}	49.82 (3)
Cu2—O2—Cu1^{i}	124.49 (9)	As1—O7—Cu3	110.54 (11)
Cu3^{ii}—O2—Cu1^{i}	152.61 (7)	As1—O7—Cu2^{viii}	66.71 (7)
Te1—O2—Cu2^{iv}	154.57 (10)	Cu3—O7—Cu2^{viii}	67.29 (6)
Cu1—O2—Cu2^{iv}	68.91 (6)	As1—O7—Cu2	55.26 (6)
Cu2—O2—Cu2^{iv}	59.50 (5)	Cu3—O7—Cu2	74.31 (6)
Cu3^{ii}—O2—Cu2^{iv}	93.94 (5)	Cu2^{viii}—O7—Cu2	88.08 (5)
Cu1^{i}—O2—Cu2^{iv}	111.78 (6)	As1—O7—Cu1^{vii}	156.06 (10)
Te1—O2—Cu3	44.72 (5)	Cu3—O7—Cu1^{vii}	88.22 (7)

Cu1—O2—Cu3	156.62 (9)	Cu2^{viii}—O7—Cu1^{vii}	136.54 (6)
Cu2—O2—Cu3	57.37 (5)	Cu2—O7—Cu1^{vii}	120.36 (6)
Cu3^{ii}—O2—Cu3	81.88 (5)	As1—O7—Cu2^{vii}	131.93 (10)
Cu1^{i}—O2—Cu3	94.51 (4)	Cu3—O7—Cu2^{vii}	51.08 (5)
Cu2^{iv}—O2—Cu3	115.82 (5)	Cu2^{viii}—O7—Cu2^{vii}	118.37 (6)
Cu3—O3—Te1	118.53 (11)	Cu2—O7—Cu2^{vii}	76.72 (4)
Cu3—O3—Cu2	141.53 (12)	Cu1^{vii}—O7—Cu2^{vii}	50.08 (3)
Te1—O3—Cu2	99.86 (9)	As1—O7—Cu1^{iii}	39.31 (6)
Cu3—O3—Cu2^{vii}	65.88 (6)	Cu3—O7—Cu1^{iii}	119.75 (8)
Te1—O3—Cu2^{vii}	90.03 (8)	Cu2^{viii}—O7—Cu1^{iii}	53.27 (3)
Cu2—O3—Cu2^{vii}	119.76 (9)	Cu2—O7—Cu1^{iii}	93.50 (5)
Cu3—O3—Cu3^{ii}	122.99 (9)	Cu1^{vii}—O7—Cu1^{iii}	141.89 (6)
Te1—O3—Cu3^{ii}	81.19 (7)	Cu2^{vii}—O7—Cu1^{iii}	167.90 (6)

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