

Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$\text{Cu}_{0.27}\text{O}_{6.37}\text{P}_{1.50}\text{Pb}_{2.23}\text{S}_0$
M_r	626.99
Crystal system, space group	Hexagonal, $P6_3/m$
Temperature (K)	300
a, c (Å)	9.8193 (1), 7.3743 (2)
V (Å ³)	615.76 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	62.05
Crystal size (mm)	0.34 × 0.08 × 0.06
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause et al., 2015)
T_{\min}, T_{\max}	0.243, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34394, 507, 486
R_{int}	0.062
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.020, 0.043, 1.32
No. of reflections	507
No. of parameters	48
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.63, -1.04

Computer programs: *SHELXL2019/1* (Sheldrick, 2019).

References

NOT FOUND

full crystallographic data

Computing details

Program(s) used to refine structure: *SHELXL2019/1* (Sheldrick, 2019).

(Pb2SO5_Cu3P_925du12h_20230814_S2)*Crystal data*

$\text{Cu}_{0.27}\text{O}_{6.37}\text{P}_{1.50}\text{Pb}_{2.23}\text{S}_0$

$M_r = 626.99$

Hexagonal, $P6_3/m$

$a = 9.8193$ (1) Å

$c = 7.3743$ (2) Å

$V = 615.76$ (2) Å³

$Z = 4$

$F(000) = 1056$

$D_x = 6.763$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9450 reflections

$\theta = 2.4\text{--}27.4^\circ$

$\mu = 62.05$ mm⁻¹

$T = 300$ K

Lump, yellow

$0.34 \times 0.08 \times 0.06$ mm

Data collection

Bruker D8 Venture Photon 100 CMOS
diffractometer

ϕ and ω scans

Absorption correction: multi-scan

(*SADABS*; Krause et al., 2015)

$T_{\min} = 0.243$, $T_{\max} = 0.746$

34394 measured reflections

507 independent reflections

486 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.062$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.4^\circ$

$h = -12 \rightarrow 12$

$k = -12 \rightarrow 12$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.020$

$wR(F^2) = 0.043$

$S = 1.32$

507 reflections

48 parameters

0 restraints

$w = 1/[\sigma^2(F_o^2) + (0.0151P)^2 + 6.0429P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.63$ e Å⁻³

$\Delta\rho_{\min} = -1.04$ e Å⁻³

Extinction correction: *SHELXL2019/1* (Sheldrick
2019), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0035 (2)

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
(*Pb2SO5_Cu3P_925du12h_20230814_S2*)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Pb1	0.333333	0.666667	0.00405 (6)	0.01133 (19)	0.880 (12)
Cu1	0.333333	0.666667	0.00405 (6)	0.01133 (19)	0.120 (12)
Pb2	0.75155 (8)	0.75165 (9)	0.250000	0.0149 (3)	0.897 (12)
Cu2	0.774 (3)	0.777 (3)	0.189 (5)	0.0149 (3)	0.051 (6)
P1	0.4006 (2)	0.3757 (2)	0.250000	0.0080 (6)	

O1A	1.000000	1.000000	0.500000	0.070 (13)	0.53 (5)
O1B	1.000000	1.000000	0.250000	0.070 (13)	0.34 (4)
O2	0.3291 (8)	0.4837 (8)	0.250000	0.015 (2)	0.96 (3)
O3	0.5843 (8)	0.4772 (8)	0.250000	0.0246 (17)	
O4	0.3492 (6)	0.2679 (6)	0.0822 (7)	0.0225 (12)	

Atomic displacement parameters (\AA^2) for (Pb2SO5_Cu3P_925du12h_20230814_S2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.0105 (2)	0.0105 (2)	0.0129 (3)	0.00527 (10)	0.000	0.000
Cu1	0.0105 (2)	0.0105 (2)	0.0129 (3)	0.00527 (10)	0.000	0.000
Pb2	0.0094 (3)	0.0087 (3)	0.0291 (5)	0.0064 (2)	0.000	0.000
Cu2	0.0094 (3)	0.0087 (3)	0.0291 (5)	0.0064 (2)	0.000	0.000
P1	0.0063 (10)	0.0029 (10)	0.0159 (11)	0.0032 (8)	0.000	0.000
O1A	0.011 (7)	0.011 (7)	0.19 (4)	0.005 (3)	0.000	0.000
O1B	0.011 (7)	0.011 (7)	0.19 (4)	0.005 (3)	0.000	0.000
O2	0.015 (4)	0.010 (4)	0.026 (4)	0.010 (3)	0.000	0.000
O3	0.009 (3)	0.020 (4)	0.039 (4)	0.004 (3)	0.000	0.000
O4	0.031 (3)	0.017 (2)	0.026 (2)	0.017 (2)	−0.007 (2)	−0.007 (2)

Geometric parameters (\AA , $^\circ$) for (Pb2SO5_Cu3P_925du12h_20230814_S2)

Pb1—O2 ⁱ	2.539 (4)	Pb2—O4 ^{vii}	2.613 (5)
Pb1—O2 ⁱⁱ	2.539 (4)	Pb2—O4 ^{viii}	2.614 (5)
Pb1—O2	2.539 (4)	Pb2—O4 ^{ix}	2.614 (5)
Pb1—O3 ⁱⁱⁱ	2.702 (5)	Cu2—Cu2 ^{vi}	0.91 (8)
Pb1—O3 ^{iv}	2.702 (5)	Cu2—O1B	2.25 (3)
Pb1—O3 ^v	2.702 (5)	Cu2—O4 ^v	2.26 (3)
Pb1—Pb1 ^{vi}	3.6275 (9)	P1—O2	1.537 (7)
Pb2—O3	2.353 (7)	P1—O4 ^{vi}	1.540 (5)
Pb2—O1B	2.4391 (8)	P1—O4	1.540 (5)
Pb2—O4 ^v	2.613 (5)	P1—O3	1.565 (7)
O2 ⁱ —Pb1—O2 ⁱⁱ	74.60 (16)	O2—P1—O4	111.6 (2)
O2 ⁱ —Pb1—O2	74.60 (16)	O4 ^{vi} —P1—O4	106.9 (4)
O2 ⁱⁱ —Pb1—O2	74.60 (16)	O2—P1—O3	109.8 (4)
O2 ⁱ —Pb1—O3 ⁱⁱⁱ	91.64 (15)	O4 ^{vi} —P1—O3	108.4 (3)
O2 ⁱⁱ —Pb1—O3 ⁱⁱⁱ	153.4 (2)	O4—P1—O3	108.4 (3)
O2—Pb1—O3 ⁱⁱⁱ	124.3 (2)	Cu2 ^x —O1B—Cu2	121.3 (3)
O2 ⁱ —Pb1—O3 ^{iv}	124.3 (2)	Cu2 ^{xi} —O1B—Cu2	116.1 (7)
O2 ⁱⁱ —Pb1—O3 ^{iv}	91.64 (15)	Cu2 ^{vi} —O1B—Cu2	23 (2)
O2—Pb1—O3 ^{iv}	153.4 (2)	Cu2 ^x —O1B—Cu2 ^{xii}	116.1 (7)
O3 ⁱⁱⁱ —Pb1—O3 ^{iv}	77.23 (17)	Cu2 ^{xi} —O1B—Cu2 ^{xii}	121.3 (3)
O2 ⁱ —Pb1—O3 ^v	153.4 (2)	Cu2 ^{vi} —O1B—Cu2 ^{xii}	116.1 (7)
O2 ⁱⁱ —Pb1—O3 ^v	124.3 (2)	Cu2—O1B—Cu2 ^{xii}	121.3 (2)
O2—Pb1—O3 ^v	91.64 (15)	Cu2 ^x —O1B—Cu2 ^{xiii}	121.3 (3)
O3 ⁱⁱⁱ —Pb1—O3 ^v	77.23 (17)	Cu2 ^{xi} —O1B—Cu2 ^{xiii}	116.1 (7)
O3 ^{iv} —Pb1—O3 ^v	77.23 (17)	Cu2 ^{vi} —O1B—Cu2 ^{xiii}	121.3 (2)
O2 ⁱ —Pb1—Pb1 ^{vi}	44.41 (10)	Cu2—O1B—Cu2 ^{xiii}	116.1 (7)
O2 ⁱⁱ —Pb1—Pb1 ^{vi}	44.41 (10)	Cu2 ^{xii} —O1B—Cu2 ^{xiii}	23 (2)
O2—Pb1—Pb1 ^{vi}	44.41 (10)	Cu2 ^x —O1B—Pb2 ^{xiii}	118.5 (5)

O3 ⁱⁱⁱ —Pb1—Pb1 ^{vi}	133.90 (11)	Cu2 ^{xi} —O1B—Pb2 ^{xiii}	118.5 (5)
O3 ^{iv} —Pb1—Pb1 ^{vi}	133.90 (11)	Cu2 ^{vi} —O1B—Pb2 ^{xiii}	120.1 (5)
O3 ^v —Pb1—Pb1 ^{vi}	133.89 (11)	Cu2—O1B—Pb2 ^{xiii}	120.1 (5)
O3—Pb2—O1B	157.18 (18)	Cu2 ^{xii} —O1B—Pb2 ^{xiii}	11.6 (10)
O3—Pb2—O4 ^v	83.91 (13)	Cu2 ^{xiii} —O1B—Pb2 ^{xiii}	11.6 (10)
O1B—Pb2—O4 ^v	103.07 (12)	Pb2 ^{xi} —O1B—Pb2 ^{xiii}	120.0
O3—Pb2—O4 ^{vii}	83.91 (13)	Pb2 ^{xi} —O1B—Pb2	120.0
O1B—Pb2—O4 ^{vii}	103.07 (12)	Pb2 ^{xiii} —O1B—Pb2	120.0
O4 ^v —Pb2—O4 ^{vii}	139.3 (2)	P1—O2—Pb1 ^{vi}	129.56 (18)
O3—Pb2—O4 ^{viii}	77.11 (19)	P1—O2—Pb1	129.56 (18)
O1B—Pb2—O4 ^{viii}	82.83 (12)	Pb1 ^{vi} —O2—Pb1	91.2 (2)
O4 ^v —Pb2—O4 ^{viii}	134.61 (17)	P1—O3—Pb2	130.7 (4)
O4 ^{vii} —Pb2—O4 ^{viii}	79.32 (10)	P1—O3—Pb1 ^v	102.6 (3)
O3—Pb2—O4 ^{ix}	77.11 (19)	Pb2—O3—Pb1 ^v	112.3 (2)
O1B—Pb2—O4 ^{ix}	82.83 (12)	P1—O3—Pb1 ^{vii}	102.6 (3)
O4 ^v —Pb2—O4 ^{ix}	79.32 (10)	Pb2—O3—Pb1 ^{vii}	112.3 (2)
O4 ^{vii} —Pb2—O4 ^{ix}	134.61 (17)	Pb1 ^v —O3—Pb1 ^{vii}	87.8 (2)
O4 ^{viii} —Pb2—O4 ^{ix}	56.5 (2)	P1—O4—Cu2 ^v	143.6 (6)
Cu2 ^{vi} —Cu2—O1B	78.4 (10)	P1—O4—Pb2 ^v	141.8 (3)
Cu2 ^{vi} —Cu2—O4 ^v	152.1 (8)	P1—O4—Pb2 ^{xiv}	98.1 (3)
O1B—Cu2—O4 ^v	122.7 (17)	Pb2 ^v —O4—Pb2 ^{xiv}	115.52 (18)
O2—P1—O4 ^{vi}	111.6 (2)		

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