**Abstract**

**Table 1**

Experimental details

| | |
|---|---|
| Crystal data | |
| Chemical formula | $Cu_{0.26}O_{6.38}P_{1.50}Pb_{2.24}S_0$ |
| $M_r$ | 628.61 |
| Crystal system, space group | Hexagonal, $P6_3/m$ |
| Temperature (K) | 300 |
| $a$, $c$ (Å) | 9.8327 (3), 7.3846 (3) |
| $V$ (Å$^3$) | 618.31 (5) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| μ (mm$^{-1}$) | 62.04 |
| Crystal size (mm) | 0.30 × 0.05 × 0.04 |
| | |
| Data collection | |
| Diffractometer | Bruker D8 Venture Photon 100 CMOS |
| Absorption correction | Multi-scan (*SADABS*; Krause et al., 2015) |
| $T_{min}$, $T_{max}$ | 0.166, 0.746 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 24230, 512, 486 |
| $R_{int}$ | 0.058 |
| $(\sin \theta/\lambda)_{max}$ (Å$^{-1}$) | 0.649 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.021, 0.044, 1.28 |
| No. of reflections | 512 |
| No. of parameters | 47 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.81, −1.01 |

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_925du24h_20230811_S1)

*Crystal data*

$Cu_{0.26}O_{6.38}P_{1.50}Pb_{2.24}S_0$
$M_r$ = 628.61
Hexagonal, $P6_3/m$
$a$ = 9.8327 (3) Å
$c$ = 7.3846 (3) Å
$V$ = 618.31 (5) Å$^3$
$Z$ = 4
$F(000)$ = 1058
$D_x$ = 6.753 Mg m$^{-3}$
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9950 reflections
θ = 2.4–27.4°
μ = 62.04 mm$^{-1}$
$T$ = 300 K
Lump, yellow
0.30 × 0.05 × 0.04 mm

*Data collection*

Bruker D8 Venture Photon 100 CMOS diffractometer
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Krause et al., 2015)
$T_{min}$ = 0.166, $T_{max}$ = 0.746
24230 measured reflections
512 independent reflections
486 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.058
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.4°
$h$ = −12→12
$k$ = −12→12
$l$ = −9→9

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.044
$S$ = 1.28
512 reflections
47 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0162P)^2 + 6.0226P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.81 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.01 e Å$^{-3}$

*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 (Å$^2$) for (Pb2SO5_Cu3P_925du24h_20230811_S1)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Pb1 | 0.333333 | 0.666667 | 0.00402 (6) | 0.01276 (17) | 0.888 (12) |
| Cu1 | 0.333333 | 0.666667 | 0.00402 (6) | 0.01276 (17) | 0.112 (12) |
| Pb2 | 0.75191 (9) | 0.75173 (10) | 0.250000 | 0.0169 (2) | 0.899 (12) |
| Cu2 | 0.777 (3) | 0.782 (4) | 0.193 (5) | 0.0169 (2) | 0.050 (6) |
| P1 | 0.4005 (3) | 0.3757 (3) | 0.250000 | 0.0093 (6) | |
| O1A | 1.000000 | 1.000000 | 0.500000 | 0.11 (2) | 0.47 (5) |

| | | | | | |
|---|---|---|---|---|---|
| O1B | 1.000000 | 1.000000 | 0.250000 | 0.11 (2) | 0.42 (5) |
| O2 | 0.3288 (8) | 0.4847 (8) | 0.250000 | 0.017 (2) | 0.95 (3) |
| O3 | 0.5847 (8) | 0.4762 (9) | 0.250000 | 0.0237 (17) | |
| O4 | 0.3486 (6) | 0.2670 (6) | 0.0824 (7) | 0.0220 (12) | |

*Atomic displacement parameters (Å²) for (Pb2SO5_Cu3P_925du24h_20230811_S1)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pb1 | 0.01388 (19) | 0.01388 (19) | 0.0105 (2) | 0.00694 (9) | 0.000 | 0.000 |
| Cu1 | 0.01388 (19) | 0.01388 (19) | 0.0105 (2) | 0.00694 (9) | 0.000 | 0.000 |
| Pb2 | 0.0123 (3) | 0.0118 (3) | 0.0288 (5) | 0.0076 (2) | 0.000 | 0.000 |
| Cu2 | 0.0123 (3) | 0.0118 (3) | 0.0288 (5) | 0.0076 (2) | 0.000 | 0.000 |
| P1 | 0.0087 (11) | 0.0070 (11) | 0.0136 (11) | 0.0050 (9) | 0.000 | 0.000 |
| O1A | 0.021 (8) | 0.021 (8) | 0.28 (6) | 0.011 (4) | 0.000 | 0.000 |
| O1B | 0.021 (8) | 0.021 (8) | 0.28 (6) | 0.011 (4) | 0.000 | 0.000 |
| O2 | 0.019 (4) | 0.014 (4) | 0.023 (4) | 0.012 (3) | 0.000 | 0.000 |
| O3 | 0.014 (3) | 0.024 (4) | 0.029 (4) | 0.006 (3) | 0.000 | 0.000 |
| O4 | 0.032 (3) | 0.019 (2) | 0.019 (2) | 0.016 (2) | −0.006 (2) | −0.007 (2) |

*Geometric parameters (Å, º) for (Pb2SO5_Cu3P_925du24h_20230811_S1)*

| | | | |
|---|---|---|---|
| Pb1—O2 | 2.534 (5) | Pb2—O4$^{viii}$ | 2.608 (5) |
| Pb1—O2$^{i}$ | 2.534 (5) | Pb2—O4$^{v}$ | 2.618 (5) |
| Pb1—O2$^{ii}$ | 2.534 (5) | Pb2—O4$^{ix}$ | 2.618 (5) |
| Pb1—O3$^{iii}$ | 2.697 (5) | Cu2—Cu2$^{vi}$ | 0.85 (8) |
| Pb1—O3$^{iv}$ | 2.697 (5) | Cu2—O1B | 2.21 (3) |
| Pb1—O3$^{v}$ | 2.697 (5) | Cu2—O4$^{v}$ | 2.30 (3) |
| Pb1—Pb1$^{vi}$ | 3.6329 (9) | P1—O4 | 1.545 (5) |
| Pb2—O3 | 2.364 (7) | P1—O4$^{vi}$ | 1.546 (5) |
| Pb2—O1B | 2.4402 (9) | P1—O2 | 1.550 (7) |
| Pb2—O4$^{vii}$ | 2.608 (5) | P1—O3 | 1.571 (7) |
| | | | |
| O2—Pb1—O2$^{i}$ | 74.29 (17) | O1B—Cu2—O4$^{v}$ | 122.8 (18) |
| O2—Pb1—O2$^{ii}$ | 74.30 (17) | O4—P1—O4$^{vi}$ | 106.4 (4) |
| O2$^{i}$—Pb1—O2$^{ii}$ | 74.30 (17) | O4—P1—O2 | 111.8 (2) |
| O2—Pb1—O3$^{iii}$ | 124.4 (2) | O4$^{vi}$—P1—O2 | 111.8 (3) |
| O2$^{i}$—Pb1—O3$^{iii}$ | 92.01 (16) | O4—P1—O3 | 108.3 (3) |
| O2$^{ii}$—Pb1—O3$^{iii}$ | 153.5 (2) | O4$^{vi}$—P1—O3 | 108.3 (3) |
| O2—Pb1—O3$^{iv}$ | 153.5 (2) | O2—P1—O3 | 110.2 (4) |
| O2$^{i}$—Pb1—O3$^{iv}$ | 124.4 (2) | Cu2—O1B—Cu2$^{x}$ | 121.2 (2) |
| O2$^{ii}$—Pb1—O3$^{iv}$ | 92.01 (16) | Cu2$^{vi}$—O1B—Cu2$^{x}$ | 116.4 (7) |
| O3$^{iii}$—Pb1—O3$^{iv}$ | 76.96 (17) | Cu2$^{xi}$—O1B—Cu2$^{x}$ | 116.4 (7) |
| O2—Pb1—O3$^{v}$ | 92.01 (16) | Cu2—O1B—Cu2$^{xii}$ | 116.4 (7) |
| O2$^{i}$—Pb1—O3$^{v}$ | 153.5 (2) | Cu2$^{vi}$—O1B—Cu2$^{xii}$ | 121.2 (2) |
| O2$^{ii}$—Pb1—O3$^{v}$ | 124.4 (2) | Cu2$^{xi}$—O1B—Cu2$^{xii}$ | 121.2 (2) |
| O3$^{iii}$—Pb1—O3$^{v}$ | 76.96 (17) | Cu2$^{x}$—O1B—Cu2$^{xii}$ | 22 (2) |
| O3$^{iv}$—Pb1—O3$^{v}$ | 76.96 (17) | Cu2$^{xiii}$—O1B—Cu2$^{xii}$ | 116.4 (7) |
| O2—Pb1—Pb1$^{vi}$ | 44.21 (11) | Pb2—O1B—Pb2$^{xiii}$ | 120.0 |
| O2$^{i}$—Pb1—Pb1$^{vi}$ | 44.21 (11) | Cu2—O1B—Pb2$^{xii}$ | 120.7 (6) |
| O2$^{ii}$—Pb1—Pb1$^{vi}$ | 44.21 (11) | Cu2$^{vi}$—O1B—Pb2$^{xii}$ | 120.7 (6) |
| O3$^{iii}$—Pb1—Pb1$^{vi}$ | 134.07 (11) | Cu2$^{xi}$—O1B—Pb2$^{xii}$ | 118.1 (6) |

| | | | |
|---|---|---|---|
| O3$^{iv}$—Pb1—Pb1$^{vi}$ | 134.07 (11) | Cu2$^{x}$—O1B—Pb2$^{xii}$ | 11.1 (10) |
| O3$^{v}$—Pb1—Pb1$^{vi}$ | 134.07 (11) | Cu2$^{xiii}$—O1B—Pb2$^{xii}$ | 118.1 (6) |
| O3—Pb2—O1B | 157.07 (18) | Cu2$^{xii}$—O1B—Pb2$^{xii}$ | 11.1 (10) |
| O3—Pb2—O4$^{vii}$ | 77.0 (2) | Pb2—O1B—Pb2$^{xii}$ | 120.0 |
| O1B—Pb2—O4$^{vii}$ | 82.85 (12) | Pb2$^{xiii}$—O1B—Pb2$^{xii}$ | 120.0 |
| O3—Pb2—O4$^{viii}$ | 77.00 (19) | P1—O2—Pb1$^{vi}$ | 129.40 (19) |
| O1B—Pb2—O4$^{viii}$ | 82.85 (12) | P1—O2—Pb1 | 129.40 (19) |
| O4$^{vii}$—Pb2—O4$^{viii}$ | 56.7 (2) | Pb1$^{vi}$—O2—Pb1 | 91.6 (2) |
| O3—Pb2—O4$^{v}$ | 84.12 (13) | P1—O3—Pb2 | 130.0 (4) |
| O1B—Pb2—O4$^{v}$ | 102.93 (12) | P1—O3—Pb1$^{v}$ | 102.9 (3) |
| O4$^{vii}$—Pb2—O4$^{v}$ | 134.78 (17) | Pb2—O3—Pb1$^{v}$ | 112.3 (2) |
| O4$^{viii}$—Pb2—O4$^{v}$ | 79.32 (9) | P1—O3—Pb1$^{ix}$ | 102.9 (3) |
| O3—Pb2—O4$^{ix}$ | 84.12 (13) | Pb2—O3—Pb1$^{ix}$ | 112.3 (2) |
| O1B—Pb2—O4$^{ix}$ | 102.93 (12) | Pb1$^{v}$—O3—Pb1$^{ix}$ | 88.1 (2) |
| O4$^{vii}$—Pb2—O4$^{ix}$ | 79.32 (9) | P1—O4—Cu2$^{v}$ | 144.2 (6) |
| O4$^{viii}$—Pb2—O4$^{ix}$ | 134.78 (17) | P1—O4—Pb2$^{xiv}$ | 98.3 (2) |
| O4$^{v}$—Pb2—O4$^{ix}$ | 139.3 (2) | P1—O4—Pb2$^{v}$ | 141.5 (3) |
| Cu2$^{vi}$—Cu2—O1B | 78.9 (11) | Pb2$^{xiv}$—O4—Pb2$^{v}$ | 115.75 (18) |
| Cu2$^{vi}$—Cu2—O4$^{v}$ | 152.1 (8) | | |

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*+*y*+1, −*x*+1, −*z*+1/2; (viii) −*x*+*y*+1, −*x*+1, *z*; (ix) −*x*+1, −*y*+1, *z*+1/2; (x) −*y*+2, *x*−*y*+1, −*z*+1/2; (xi) −*x*+*y*+1, −*x*+2, −*z*+1/2; (xii) −*y*+2, *x*−*y*+1, *z*; (xiii) −*x*+*y*+1, −*x*+2, *z*; (xiv) −*y*+1, *x*−*y*, *z*.