Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dilanthanum copper indium pentaselenide, $La_2CuInSe_5$

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Received 27 August 2007; accepted 19 September 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(Se–Cu) = 0.001 Å; R factor = 0.020; wR factor = 0.041; data-to-parameter ratio = 20.2.

Single crystals of $La_2CuInSe_5$ were obtained by sintering a La_2Se_3–Cu_2Se—In_2Se_3 mixture. The crystal structure is similar to the previously reported La_2CuInS_5. The coordination polyhedron of the Cu atom is a trigonal bipyramid. In contrast to the La_2CuInS_5 compound, the position of this atom is fully occupied and ordered.

Related literature

For the related La_2CuInS_5 structure, see Huch, Gulay, Olekseyuk & Pietraszko (2007). For a previous structure determination of the title compound from powder data, see Huch, Gulay & Olekseyuk (2007). For crystallographic tools, see Spek (2003).

Experimental

Crystal data

$La_2CuInSe_5$
M_r = 850.98
Orthorhombic, *Pnma*
a = 12.051 (2) Å
b = 4.1223 (8) Å
c = 17.580 (4) Å
V = 873.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 35.34 mm^{-1}
T = 295 (2) K
0.13 × 0.07 × 0.03 mm

Data collection

Kuma KM-4 diffractometer with CCD detector
Absorption correction: numerical (*CrysAlis RED*; Mayer, 2006)
T_{min} = 0.076, T_{max} = 0.396
9371 measured reflections
1134 independent reflections
1049 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.041
S = 1.12
1134 reflections
56 parameters
$\Delta\rho_{max}$ = 2.03 e Å^{-3}
$\Delta\rho_{min}$ = −1.68 e Å^{-3}

Table 1
Selected bond lengths (Å).

La1—Se1^{i}	3.1094 (7)	La2—Se5^{iv}	3.0323 (7)
La1—Se2	3.3013 (9)	In1—Se4^{vii}	2.6754 (9)
La1—Se2^{ii}	3.2669 (10)	In1—Se1	2.6972 (9)
La1—Se4^{iii}	3.0714 (7)	In1—Se2^{v}	2.7061 (6)
La1—Se5^{iv}	3.0482 (7)	In1—Se3^{viii}	2.9079 (7)
La2—Se2	3.3763 (9)	Cu1—Se1	2.6479 (13)
La2—Se3^{v}	3.0988 (7)	Cu1—Se1^{iii}	2.4443 (7)
La2—Se3^{vi}	3.1407 (9)	Cu1—Se1^{i}	2.4443 (7)
La2—Se4^{iv}	3.0969 (6)	Cu1—Se5^{ix}	2.3920 (12)

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x+\frac{1}{2}, y, -z+\frac{3}{2}$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+\frac{1}{2}, -y, z+\frac{1}{2}$; (v) $-x+\frac{1}{2}, -y, z-\frac{1}{2}$; (vi) $x-\frac{1}{2}, y, -z+\frac{3}{2}$; (vii) $x-\frac{1}{2}, y, -z+\frac{1}{2}$; (viii) $-x+\frac{1}{2}, -y+1, z-\frac{1}{2}$; (ix) $x+\frac{1}{2}, y, -z+\frac{1}{2}$.

Data collection: *CrysAlis CCD* (Mayer, 2006); cell refinement: *CrysAlis RED* (Mayer, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *publCIF* (Westrip, 2007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2045).

References

Brandenburg, K. (2005). *DIAMOND*. Release 3.0e. Crystal Impact GbR, Bonn, Germany.
Huch, M. R., Gulay, L. D. & Olekseyuk, I. D. (2007). *J. Alloys Compd*, **439**, 156–161.
Huch, M. R., Gulay, L. D., Olekseyuk, I. D. & Pietraszko, A. (2007). *J. Alloys Compd*, **425**, 230–234.
Mayer, M. (2006). *CrysAlis CCD* (Version 1.171.10) and *CrysAlis RED* (Version 1.171.38.1). Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Westrip (2007). *publCIF*. In preparation.

  doi:10.1107/S1600536807046041

supplementary materials

Acta Cryst. (2007). E**63**, i182 [**doi:10.1107/S1600536807046041**]

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Comment

The formation of quaternary $La_2CuInSe_5$ had been established earlier during the investigation of the phase relations in the La_2Se_3—Cu_2Se—In_2Se_3 system (Huch, Gulay & Olekseyuk, 2007) and the crystal structure of this compound was investigated using X-ray powder diffraction (space group *Pnma*). The crystal structure of $La_2CuInSe_5$ has been reinvestigated by means of X-ray single-crystal diffraction and presented here. Crystal structure of the title compound is similar to previously reported La_2CuInS_5 (Huch, Gulay, Olekseyuk & Pietraszko, 2007).

The unit cell and the coordination polyhedra of the La, Cu, In and Se atoms in the structure of the $La_2CuInSe_5$ compound are shown in Fig. 1. Selenium atoms create bi-capped trigonal prisms, octahedra and tetrahedra around the La, In and Cu atoms, respectively. The coordination polyhedron of the copper atom can be extended to a trigonal bipyramid. In contrast to La_2CuInS_5, the position of the Cu atom is fully occupied and ordered (Fig. 2). The single-crystal data for $La_2CuInSe_5$ agree well with our previous powder diffraction results (Huch, Gulay & Olekseyuk, 2007).

Experimental

The sample with the nominal compositions $La_2CuInSe_5$ was prepared by sintering the elemental constituents (purchased from Alfa Aesar) of the purity better than 99.9 wt.% in an evacuated quartz ampoule. The synthesis was realised in a tube furnace. The ampoule was heated with a heating rate of 30 K/h to maximal temperature 1420 K. The samples were kept at this temperature during 3 h. Afterwards they were cooled slowly (10 K/h) to 870 K and annealed at this temperature during 240 h. After annealing the ampoule with the sample was quenched in cold water. An EDAX PV9800 microanalyzer was used for the confirmation of the compositions of the crystals. Calculated for $La_2CuInSe_5$ (black crystals) % La: 32.65, Cu: 7.47, In: 13.49, Se: 46.39 and found % La: 31.74, Cu: 7.57, In: 13.65, Se: 47.04.

Refinement

The crystal structure was solved by Patterson methods (Sheldrick, 1997) and refined by full matrix least squares method using *SHELXL97* (Sheldrick, 1997). Space group *Pnma* was confirmed with *PLATON* (Spek, 2003) and no additional symmetry elements were found. The highest peak and deepest hole in the Fourier map are found 0.94Å and 0.65 Å, respectively, from Cu1.

Figures

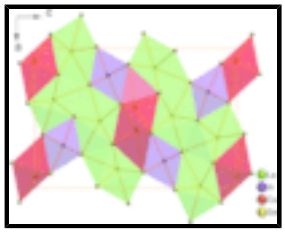


Fig. 1. The packing of $La_2CuInSe_5$ viewed along the *b* axis.

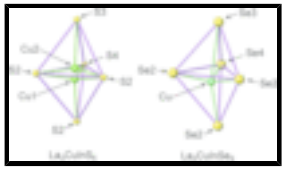


Fig. 2. Trigonal bi-pyramids around the Cu atom in the structures of La_2CuInS_5 and $La_2CuInSe_5$.

dilanthanum copper indium pentaselenide

Crystal data

$La_2CuInSe_5$	F_{000} = 1448
M_r = 850.98	D_x = 6.472 Mg m^{-3}
Orthorhombic, *Pnma*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2n	Cell parameters from 1049 reflections
a = 12.051 (2) Å	θ = 2.9–27.5º
b = 4.1223 (8) Å	μ = 35.34 mm^{-1}
c = 17.580 (4) Å	*T* = 295 (2) K
V = 873.3 (3) Å^3	Prism, black
Z = 4	0.13 × 0.07 × 0.03 mm

Data collection

Kuma KM-4 diffractometer with CCD detector	1134 independent reflections
Radiation source: fine-focus sealed tube	1049 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
Detector resolution: 33.133 pixels mm^{-1}	θ_{max} = 27.5º
T = 295(2) K	θ_{min} = 2.9º
ω scans	*h* = −15→15
Absorption correction: numerical (CrysAlis RED; Mayer, 2006)	*k* = −5→4
T_{min} = 0.076, T_{max} = 0.396	*l* = −22→22
9371 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0208P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.020$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.041$	$\Delta\rho_{max} = 2.03$ e Å^{-3}
$S = 1.12$	$\Delta\rho_{min} = -1.68$ e Å^{-3}
1134 reflections	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
56 parameters	Extinction coefficient: 0.00141 (8)
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
La1	0.47993 (3)	0.2500	0.67902 (2)	0.00840 (10)
La2	0.13680 (3)	0.2500	0.59252 (2)	0.00889 (10)
In1	0.19371 (4)	0.2500	0.35994 (3)	0.01362 (12)
Cu1	0.58400 (8)	0.2500	0.50300 (5)	0.0222 (2)
Se1	0.39751 (5)	0.2500	0.42335 (4)	0.00954 (15)
Se2	0.24095 (5)	0.2500	0.77082 (4)	0.01086 (15)
Se3	0.38864 (5)	0.2500	0.96206 (4)	0.00997 (15)
Se4	0.48589 (5)	0.2500	0.19359 (4)	0.00883 (15)
Se5	0.18170 (5)	0.2500	0.11544 (4)	0.00930 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.00886 (19)	0.00760 (19)	0.00873 (19)	0.000	−0.00046 (13)	0.000
La2	0.00796 (19)	0.00757 (19)	0.0111 (2)	0.000	0.00015 (14)	0.000
In1	0.0104 (2)	0.0147 (2)	0.0158 (3)	0.000	−0.00293 (18)	0.000
Cu1	0.0312 (6)	0.0196 (5)	0.0159 (5)	0.000	0.0037 (4)	0.000
Se1	0.0082 (3)	0.0098 (3)	0.0106 (3)	0.000	−0.0007 (2)	0.000
Se2	0.0107 (3)	0.0117 (3)	0.0101 (3)	0.000	−0.0002 (2)	0.000
Se3	0.0104 (3)	0.0102 (3)	0.0093 (3)	0.000	0.0010 (2)	0.000
Se4	0.0093 (3)	0.0090 (3)	0.0082 (3)	0.000	−0.0004 (2)	0.000
Se5	0.0074 (3)	0.0088 (3)	0.0118 (3)	0.000	0.0009 (2)	0.000

Geometric parameters (Å, °)

La1—Se1^{i}	3.1094 (7)	Cu1—Se1^{ii}	2.4443 (7)
La1—Se1^{ii}	3.1094 (7)	Cu1—Se1^{i}	2.4443 (7)
La1—Se2	3.3013 (9)	Cu1—Se5^{xii}	2.3920 (12)
La1—Se2^{iii}	3.2669 (10)	Cu1—Cu1^{i}	2.8911 (14)
La1—Se4^{ii}	3.0714 (7)	Cu1—Cu1^{ii}	2.8911 (14)
La1—Se4^{i}	3.0714 (7)	Se1—Cu1^{ii}	2.4443 (7)
La1—Se5^{iv}	3.0482 (7)	Se1—Cu1^{i}	2.4443 (7)
La1—Se5^{v}	3.0482 (7)	Se1—La1^{i}	3.1094 (7)
La1—Cu1	3.3389 (12)	Se1—La1^{ii}	3.1094 (7)
La1—La1^{vi}	4.1223 (8)	Se2—In1^{v}	2.7061 (6)
La1—La1^{vii}	4.1223 (8)	Se2—In1^{iv}	2.7061 (6)
La2—Se2	3.3763 (9)	Se2—La1^{x}	3.2669 (10)
La2—Se3^{viii}	3.0988 (7)	Se3—In1^{iv}	2.9079 (7)
La2—Se3^{ix}	3.0988 (7)	Se3—In1^{v}	2.9079 (7)
La2—Se3^{x}	3.1407 (9)	Se3—La2^{v}	3.0988 (7)
La2—Se4^{v}	3.0969 (7)	Se3—La2^{iv}	3.0988 (7)
La2—Se4^{iv}	3.0969 (6)	Se3—La2^{iii}	3.1407 (9)
La2—Se5^{v}	3.0323 (7)	Se4—In1^{xii}	2.6754 (9)
La2—Se5^{iv}	3.0323 (7)	Se4—La1^{ii}	3.0714 (7)
La2—La2^{vi}	4.1223 (8)	Se4—La1^{i}	3.0714 (7)
La2—La2^{vii}	4.1223 (8)	Se4—La2^{viii}	3.0969 (6)
In1—Se4^{xi}	2.6754 (9)	Se4—La2^{ix}	3.0969 (6)
In1—Se1	2.6972 (9)	Se5—Cu1^{xi}	2.3920 (12)
In1—Se2^{viii}	2.7061 (6)	Se5—La2^{ix}	3.0323 (7)
In1—Se2^{ix}	2.7061 (6)	Se5—La2^{viii}	3.0323 (7)
In1—Se3^{ix}	2.9079 (7)	Se5—La1^{viii}	3.0482 (7)
In1—Se3^{viii}	2.9079 (7)	Se5—La1^{ix}	3.0482 (7)
Cu1—Se1	2.6479 (13)		
Se5^{iv}—La1—Se5^{v}	85.09 (2)	Se3^{ix}—La2—La2^{vii}	131.694 (12)
Se5^{iv}—La1—Se4^{ii}	143.79 (2)	Se3^{x}—La2—La2^{vii}	90.0
Se5^{v}—La1—Se4^{ii}	84.221 (18)	Se2—La2—La2^{vii}	90.0
Se5^{iv}—La1—Se4^{i}	84.221 (18)	La2^{vi}—La2—La2^{vii}	180.00 (2)
Se5^{v}—La1—Se4^{i}	143.79 (2)	Se4^{xi}—In1—Se1	176.18 (3)
Se4^{ii}—La1—Se4^{i}	84.30 (2)	Se4^{xi}—In1—Se2^{viii}	93.94 (2)
Se5^{iv}—La1—Se1^{i}	69.09 (2)	Se1—In1—Se2^{viii}	88.53 (2)
Se5^{v}—La1—Se1^{i}	122.65 (2)	Se4^{xi}—In1—Se2^{ix}	93.94 (2)
Se4^{ii}—La1—Se1^{i}	143.43 (2)	Se1—In1—Se2^{ix}	88.53 (2)
Se4^{i}—La1—Se1^{i}	85.03 (2)	Se2^{viii}—In1—Se2^{ix}	99.22 (3)

Se5^{iv}—La1—Se1^{ii}	122.65 (2)	Se4^{xi}—In1—Se3^{ix}	84.12 (2)
Se5^{v}—La1—Se1^{ii}	69.09 (2)	Se1—In1—Se3^{ix}	93.19 (2)
Se4^{ii}—La1—Se1^{ii}	85.03 (2)	Se2^{viii}—In1—Se3^{ix}	175.27 (2)
Se4^{i}—La1—Se1^{ii}	143.43 (2)	Se2^{ix}—In1—Se3^{ix}	85.23 (2)
Se1^{i}—La1—Se1^{ii}	83.04 (2)	Se4^{xi}—In1—Se3^{viii}	84.12 (2)
Se5^{iv}—La1—Se2^{iii}	135.583 (13)	Se1—In1—Se3^{viii}	93.19 (2)
Se5^{v}—La1—Se2^{iii}	135.583 (13)	Se2^{viii}—In1—Se3^{viii}	85.23 (2)
Se4^{ii}—La1—Se2^{iii}	70.975 (16)	Se2^{ix}—In1—Se3^{viii}	175.27 (2)
Se4^{i}—La1—Se2^{iii}	70.975 (16)	Se3^{ix}—In1—Se3^{viii}	90.28 (3)
Se1^{i}—La1—Se2^{iii}	72.473 (18)	Se5^{xii}—Cu1—Se1^{ii}	114.60 (3)
Se1^{ii}—La1—Se2^{iii}	72.473 (18)	Se5^{xii}—Cu1—Se1^{i}	114.60 (3)
Se5^{iv}—La1—Se2	67.777 (19)	Se1^{ii}—Cu1—Se1^{i}	114.97 (5)
Se5^{v}—La1—Se2	67.777 (19)	Se5^{xii}—Cu1—Se1	87.56 (4)
Se4^{ii}—La1—Se2	76.149 (19)	Se1^{ii}—Cu1—Se1	110.95 (3)
Se4^{i}—La1—Se2	76.149 (19)	Se1^{i}—Cu1—Se1	110.95 (3)
Se1^{i}—La1—Se2	134.211 (13)	Se5^{xii}—Cu1—Cu1^{i}	108.24 (4)
Se1^{ii}—La1—Se2	134.211 (13)	Se1^{ii}—Cu1—Cu1^{i}	133.18 (6)
Se2^{iii}—La1—Se2	135.077 (17)	Se1^{i}—Cu1—Cu1^{i}	58.80 (2)
Se5^{iv}—La1—Cu1	84.27 (2)	Se1—Cu1—Cu1^{i}	52.15 (3)
Se5^{v}—La1—Cu1	84.27 (2)	Se5^{xii}—Cu1—Cu1^{ii}	108.24 (4)
Se4^{ii}—La1—Cu1	128.709 (18)	Se1^{ii}—Cu1—Cu1^{ii}	58.80 (2)
Se4^{i}—La1—Cu1	128.709 (18)	Se1^{i}—Cu1—Cu1^{ii}	133.18 (6)
Se1^{i}—La1—Cu1	44.373 (13)	Se1—Cu1—Cu1^{ii}	52.15 (3)
Se1^{ii}—La1—Cu1	44.373 (13)	Cu1^{i}—Cu1—Cu1^{ii}	90.95 (6)
Se2^{iii}—La1—Cu1	83.60 (2)	Se5^{xii}—Cu1—La1	172.58 (4)
Se2—La1—Cu1	141.33 (2)	Se1^{ii}—Cu1—La1	62.83 (3)
Se5^{iv}—La1—La1^{vi}	132.546 (12)	Se1^{i}—Cu1—La1	62.83 (3)
Se5^{v}—La1—La1^{vi}	47.454 (12)	Se1—Cu1—La1	99.86 (4)
Se4^{ii}—La1—La1^{vi}	47.849 (12)	Cu1^{i}—Cu1—La1	76.75 (4)
Se4^{i}—La1—La1^{vi}	132.151 (12)	Cu1^{ii}—Cu1—La1	76.75 (4)
Se1^{i}—La1—La1^{vi}	131.520 (11)	Cu1^{ii}—Se1—Cu1^{i}	114.97 (5)
Se1^{ii}—La1—La1^{vi}	48.480 (11)	Cu1^{ii}—Se1—Cu1	69.05 (3)
Se2^{iii}—La1—La1^{vi}	90.0	Cu1^{i}—Se1—Cu1	69.05 (3)
Se2—La1—La1^{vi}	90.0	Cu1^{ii}—Se1—In1	107.57 (3)
Cu1—La1—La1^{vi}	90.0	Cu1^{i}—Se1—In1	107.57 (3)
Se5^{iv}—La1—La1^{vii}	47.454 (12)	Cu1—Se1—In1	172.49 (4)
Se5^{v}—La1—La1^{vii}	132.546 (12)	Cu1^{ii}—Se1—La1^{i}	145.31 (3)
Se4^{ii}—La1—La1^{vii}	132.151 (12)	Cu1^{i}—Se1—La1^{i}	72.80 (3)
Se4^{i}—La1—La1^{vii}	47.849 (12)	Cu1—Se1—La1^{i}	84.43 (2)
Se1^{i}—La1—La1^{vii}	48.480 (11)	In1—Se1—La1^{i}	101.15 (2)
Se1^{ii}—La1—La1^{vii}	131.520 (11)	Cu1^{ii}—Se1—La1^{ii}	72.80 (3)

Se2^{iii}—La1—La1^{vii}	90.0	Cu1^{i}—Se1—La1^{ii}	145.31 (3)
Se2—La1—La1^{vii}	90.0	Cu1—Se1—La1^{ii}	84.43 (2)
Cu1—La1—La1^{vii}	90.0	In1—Se1—La1^{ii}	101.15 (2)
La1^{vi}—La1—La1^{vii}	180.00 (2)	La1^{i}—Se1—La1^{ii}	83.04 (2)
Se5^{v}—La2—Se5^{iv}	85.65 (2)	In1^{v}—Se2—In1^{iv}	99.22 (3)
Se5^{v}—La2—Se4^{v}	79.38 (2)	In1^{v}—Se2—La1^{x}	97.12 (2)
Se5^{iv}—La2—Se4^{v}	136.10 (2)	In1^{iv}—Se2—La1^{x}	97.12 (2)
Se5^{v}—La2—Se4^{iv}	136.10 (2)	In1^{v}—Se2—La1	91.67 (2)
Se5^{iv}—La2—Se4^{iv}	79.382 (19)	In1^{iv}—Se2—La1	91.67 (2)
Se4^{v}—La2—Se4^{iv}	83.45 (2)	La1^{x}—Se2—La1	166.40 (2)
Se5^{v}—La2—Se3^{viii}	128.45 (2)	In1^{v}—Se2—La2	130.213 (15)
Se5^{iv}—La2—Se3^{viii}	73.595 (18)	In1^{iv}—Se2—La2	130.213 (15)
Se4^{v}—La2—Se3^{viii}	145.09 (2)	La1^{x}—Se2—La2	83.84 (2)
Se4^{iv}—La2—Se3^{viii}	86.26 (2)	La1—Se2—La2	82.56 (2)
Se5^{v}—La2—Se3^{ix}	73.595 (18)	In1^{iv}—Se3—In1^{v}	90.28 (3)
Se5^{iv}—La2—Se3^{ix}	128.45 (2)	In1^{iv}—Se3—La2^{v}	153.46 (3)
Se4^{v}—La2—Se3^{ix}	86.26 (2)	In1^{v}—Se3—La2^{v}	87.232 (18)
Se4^{iv}—La2—Se3^{ix}	145.09 (2)	In1^{iv}—Se3—La2^{iv}	87.232 (18)
Se3^{viii}—La2—Se3^{ix}	83.39 (2)	In1^{v}—Se3—La2^{iv}	153.46 (3)
Se5^{v}—La2—Se3^{x}	136.672 (12)	La2^{v}—Se3—La2^{iv}	83.39 (2)
Se5^{iv}—La2—Se3^{x}	136.672 (12)	In1^{iv}—Se3—La2^{iii}	97.84 (2)
Se4^{v}—La2—Se3^{x}	73.779 (19)	In1^{v}—Se3—La2^{iii}	97.84 (2)
Se4^{iv}—La2—Se3^{x}	73.779 (19)	La2^{v}—Se3—La2^{iii}	108.680 (18)
Se3^{viii}—La2—Se3^{x}	71.320 (18)	La2^{iv}—Se3—La2^{iii}	108.680 (18)
Se3^{ix}—La2—Se3^{x}	71.320 (18)	In1^{xii}—Se4—La1^{ii}	97.52 (2)
Se5^{v}—La2—Se2	66.952 (16)	In1^{xii}—Se4—La1^{i}	97.52 (2)
Se5^{iv}—La2—Se2	66.952 (16)	La1^{ii}—Se4—La1^{i}	84.30 (2)
Se4^{v}—La2—Se2	69.200 (18)	In1^{xii}—Se4—La2^{viii}	104.19 (2)
Se4^{iv}—La2—Se2	69.200 (18)	La1^{ii}—Se4—La2^{viii}	158.28 (3)
Se3^{viii}—La2—Se2	136.374 (13)	La1^{i}—Se4—La2^{viii}	92.046 (16)
Se3^{ix}—La2—Se2	136.374 (13)	In1^{xii}—Se4—La2^{ix}	104.19 (2)
Se3^{x}—La2—Se2	129.61 (2)	La1^{ii}—Se4—La2^{ix}	92.046 (16)
Se5^{v}—La2—La2^{vi}	47.177 (12)	La1^{i}—Se4—La2^{ix}	158.28 (3)
Se5^{iv}—La2—La2^{vi}	132.823 (12)	La2^{viii}—Se4—La2^{ix}	83.45 (2)
Se4^{v}—La2—La2^{vi}	48.276 (11)	Cu1^{xi}—Se5—La2^{ix}	103.85 (3)
Se4^{iv}—La2—La2^{vi}	131.724 (11)	Cu1^{xi}—Se5—La2^{viii}	103.85 (3)
Se3^{viii}—La2—La2^{vi}	131.694 (12)	La2^{ix}—Se5—La2^{viii}	85.65 (2)
Se3^{ix}—La2—La2^{vi}	48.306 (12)	Cu1^{xi}—Se5—La1^{viii}	90.27 (3)
Se3^{x}—La2—La2^{vi}	90.0	La2^{ix}—Se5—La1^{viii}	165.76 (3)
Se2—La2—La2^{vi}	90.0	La2^{viii}—Se5—La1^{viii}	92.868 (17)
Se5^{v}—La2—La2^{vii}	132.823 (12)	Cu1^{xi}—Se5—La1^{ix}	90.27 (3)

Se5^{iv}—La2—La2^{vii}	47.177 (12)	La2^{ix}—Se5—La1^{ix}	92.868 (17)
Se4^{v}—La2—La2^{vii}	131.724 (11)	La2^{viii}—Se5—La1^{ix}	165.76 (3)
Se4^{iv}—La2—La2^{vii}	48.276 (11)	La1^{viii}—Se5—La1^{ix}	85.09 (2)
Se3^{viii}—La2—La2^{vii}	48.306 (12)		
Se5^{iv}—La1—Cu1—Se1^{ii}	151.39 (3)	Se2^{viii}—In1—Se1—La1^{i}	7.132 (18)
Se5^{v}—La1—Cu1—Se1^{ii}	65.77 (3)	Se2^{ix}—In1—Se1—La1^{i}	−92.14 (2)
Se4^{ii}—La1—Cu1—Se1^{ii}	−12.10 (4)	Se3^{ix}—In1—Se1—La1^{i}	−177.276 (16)
Se4^{i}—La1—Cu1—Se1^{ii}	−130.74 (3)	Se3^{viii}—In1—Se1—La1^{i}	92.27 (2)
Se1^{i}—La1—Cu1—Se1^{ii}	−142.84 (5)	Se2^{viii}—In1—Se1—La1^{ii}	92.14 (2)
Se2^{iii}—La1—Cu1—Se1^{ii}	−71.42 (2)	Se2^{ix}—In1—Se1—La1^{ii}	−7.132 (18)
Se2—La1—Cu1—Se1^{ii}	108.58 (2)	Se3^{ix}—In1—Se1—La1^{ii}	−92.27 (2)
La1^{vi}—La1—Cu1—Se1^{ii}	18.58 (2)	Se3^{viii}—In1—Se1—La1^{ii}	177.276 (16)
La1^{vii}—La1—Cu1—Se1^{ii}	−161.42 (2)	Se5^{iv}—La1—Se2—In1^{v}	−177.282 (19)
Se5^{iv}—La1—Cu1—Se1^{i}	−65.77 (3)	Se5^{v}—La1—Se2—In1^{v}	−83.44 (2)
Se5^{v}—La1—Cu1—Se1^{i}	−151.39 (3)	Se4^{ii}—La1—Se2—In1^{v}	5.917 (15)
Se4^{ii}—La1—Cu1—Se1^{i}	130.74 (3)	Se4^{i}—La1—Se2—In1^{v}	93.36 (2)
Se4^{i}—La1—Cu1—Se1^{i}	12.10 (4)	Se1^{i}—La1—Se2—In1^{v}	162.00 (2)
Se1^{ii}—La1—Cu1—Se1^{i}	142.84 (5)	Se1^{ii}—La1—Se2—In1^{v}	−62.72 (3)
Se2^{iii}—La1—Cu1—Se1^{i}	71.42 (2)	Se2^{iii}—La1—Se2—In1^{v}	49.641 (15)
Se2—La1—Cu1—Se1^{i}	−108.58 (2)	Cu1—La1—Se2—In1^{v}	−130.359 (15)
La1^{vi}—La1—Cu1—Se1^{i}	161.42 (2)	La1^{vi}—La1—Se2—In1^{v}	−40.359 (15)
La1^{vii}—La1—Cu1—Se1^{i}	−18.58 (2)	La1^{vii}—La1—Se2—In1^{v}	139.641 (15)
Se5^{iv}—La1—Cu1—Se1	42.810 (12)	Se5^{iv}—La1—Se2—In1^{iv}	83.44 (2)
Se5^{v}—La1—Cu1—Se1	−42.810 (12)	Se5^{v}—La1—Se2—In1^{iv}	177.282 (19)
Se4^{ii}—La1—Cu1—Se1	−120.68 (2)	Se4^{ii}—La1—Se2—In1^{iv}	−93.36 (2)
Se4^{i}—La1—Cu1—Se1	120.68 (2)	Se4^{i}—La1—Se2—In1^{iv}	−5.917 (15)
Se1^{i}—La1—Cu1—Se1	108.58 (2)	Se1^{i}—La1—Se2—In1^{iv}	62.72 (3)
Se1^{ii}—La1—Cu1—Se1	−108.58 (2)	Se1^{ii}—La1—Se2—In1^{iv}	−162.00 (2)
Se2^{iii}—La1—Cu1—Se1	180.0	Se2^{iii}—La1—Se2—In1^{iv}	−49.641 (15)
Se2—La1—Cu1—Se1	0.0	Cu1—La1—Se2—In1^{iv}	130.359 (15)
Se5^{iv}—La1—Cu1—Cu1^{i}	−4.28 (3)	La1^{vi}—La1—Se2—In1^{iv}	−139.641 (15)
Se5^{v}—La1—Cu1—Cu1^{i}	−89.90 (3)	La1^{vii}—La1—Se2—In1^{iv}	40.359 (15)
Se4^{ii}—La1—Cu1—Cu1^{i}	−167.78 (2)	Se5^{iv}—La1—Se2—La1^{x}	−46.923 (13)
Se4^{i}—La1—Cu1—Cu1^{i}	73.59 (4)	Se5^{v}—La1—Se2—La1^{x}	46.923 (13)
Se1^{i}—La1—Cu1—Cu1^{i}	61.49 (2)	Se4^{ii}—La1—Se2—La1^{x}	136.276 (12)
Se1^{ii}—La1—Cu1—Cu1^{i}	−155.67 (5)	Se4^{i}—La1—Se2—La1^{x}	−136.276 (12)
Se2^{iii}—La1—Cu1—Cu1^{i}	132.91 (3)	Se1^{i}—La1—Se2—La1^{x}	−67.64 (2)
Se2—La1—Cu1—Cu1^{i}	−47.09 (3)	Se1^{ii}—La1—Se2—La1^{x}	67.64 (2)
La1^{vi}—La1—Cu1—Cu1^{i}	−137.09 (3)	Se2^{iii}—La1—Se2—La1^{x}	180.0
La1^{vii}—La1—Cu1—Cu1^{i}	42.91 (3)	Cu1—La1—Se2—La1^{x}	0.0

Se5^{iv}—La1—Cu1—Cu1^{ii}	89.90 (3)	Se5^{iv}—La1—Se2—La2	−46.923 (13)
Se5^{v}—La1—Cu1—Cu1^{ii}	4.28 (3)	Se5^{v}—La1—Se2—La2	46.923 (13)
Se4^{ii}—La1—Cu1—Cu1^{ii}	−73.59 (4)	Se4^{ii}—La1—Se2—La2	136.276 (12)
Se4^{i}—La1—Cu1—Cu1^{ii}	167.78 (2)	Se4^{i}—La1—Se2—La2	−136.276 (12)
Se1^{i}—La1—Cu1—Cu1^{ii}	155.67 (5)	Se1^{i}—La1—Se2—La2	−67.64 (2)
Se1^{ii}—La1—Cu1—Cu1^{ii}	−61.49 (2)	Se1^{ii}—La1—Se2—La2	67.64 (2)
Se2^{iii}—La1—Cu1—Cu1^{ii}	−132.91 (3)	Se2^{iii}—La1—Se2—La2	180.0
Se2—La1—Cu1—Cu1^{ii}	47.09 (3)	Cu1—La1—Se2—La2	0.0
La1^{vi}—La1—Cu1—Cu1^{ii}	−42.91 (3)	Se5^{v}—La2—Se2—In1^{v}	38.26 (3)
La1^{vii}—La1—Cu1—Cu1^{ii}	137.09 (3)	Se5^{iv}—La2—Se2—In1^{v}	133.50 (4)
Se5^{xii}—Cu1—Se1—Cu1^{ii}	−115.45 (3)	Se4^{v}—La2—Se2—In1^{v}	−48.73 (3)
Se1^{ii}—Cu1—Se1—Cu1^{ii}	0.0	Se4^{iv}—La2—Se2—In1^{v}	−139.52 (4)
Se1^{i}—Cu1—Se1—Cu1^{ii}	129.09 (6)	Se3^{viii}—La2—Se2—In1^{v}	160.47 (3)
Cu1^{i}—Cu1—Se1—Cu1^{ii}	129.09 (6)	Se3^{ix}—La2—Se2—In1^{v}	11.28 (5)
La1—Cu1—Se1—Cu1^{ii}	64.55 (3)	Se3^{x}—La2—Se2—In1^{v}	−94.12 (3)
Se5^{xii}—Cu1—Se1—Cu1^{i}	115.45 (3)	La2^{vi}—La2—Se2—In1^{v}	−4.12 (3)
Se1^{ii}—Cu1—Se1—Cu1^{i}	−129.09 (6)	La2^{vii}—La2—Se2—In1^{v}	175.88 (3)
Se1^{i}—Cu1—Se1—Cu1^{i}	0.0	Se5^{v}—La2—Se2—In1^{iv}	−133.50 (4)
Cu1^{ii}—Cu1—Se1—Cu1^{i}	−129.09 (6)	Se5^{iv}—La2—Se2—In1^{iv}	−38.26 (3)
La1—Cu1—Se1—Cu1^{i}	−64.55 (3)	Se4^{v}—La2—Se2—In1^{iv}	139.52 (4)
Se5^{xii}—Cu1—Se1—La1^{i}	41.761 (11)	Se4^{iv}—La2—Se2—In1^{iv}	48.73 (3)
Se1^{ii}—Cu1—Se1—La1^{i}	157.22 (3)	Se3^{viii}—La2—Se2—In1^{iv}	−11.28 (5)
Se1^{i}—Cu1—Se1—La1^{i}	−73.69 (3)	Se3^{ix}—La2—Se2—In1^{iv}	−160.47 (3)
Cu1^{i}—Cu1—Se1—La1^{i}	−73.69 (3)	Se3^{x}—La2—Se2—In1^{iv}	94.12 (3)
Cu1^{ii}—Cu1—Se1—La1^{i}	157.22 (3)	La2^{vi}—La2—Se2—In1^{iv}	−175.88 (3)
La1—Cu1—Se1—La1^{i}	−138.239 (11)	La2^{vii}—La2—Se2—In1^{iv}	4.12 (3)
Se5^{xii}—Cu1—Se1—La1^{ii}	−41.761 (11)	Se5^{v}—La2—Se2—La1^{x}	132.380 (13)
Se1^{ii}—Cu1—Se1—La1^{ii}	73.69 (3)	Se5^{iv}—La2—Se2—La1^{x}	−132.380 (13)
Se1^{i}—Cu1—Se1—La1^{ii}	−157.22 (3)	Se4^{v}—La2—Se2—La1^{x}	45.394 (13)
Cu1^{i}—Cu1—Se1—La1^{ii}	−157.22 (3)	Se4^{iv}—La2—Se2—La1^{x}	−45.394 (13)
Cu1^{ii}—Cu1—Se1—La1^{ii}	73.69 (3)	Se3^{viii}—La2—Se2—La1^{x}	−105.41 (3)
La1—Cu1—Se1—La1^{ii}	138.239 (11)	Se3^{ix}—La2—Se2—La1^{x}	105.41 (3)
Se2^{viii}—In1—Se1—Cu1^{ii}	167.44 (3)	Se3^{x}—La2—Se2—La1^{x}	0.0
Se2^{ix}—In1—Se1—Cu1^{ii}	68.17 (3)	Se5^{v}—La2—Se2—La1	−47.620 (13)
Se3^{ix}—In1—Se1—Cu1^{ii}	−16.97 (3)	Se5^{iv}—La2—Se2—La1	47.620 (13)
Se3^{viii}—In1—Se1—Cu1^{ii}	−107.42 (3)	Se4^{v}—La2—Se2—La1	−134.606 (13)
Se2^{viii}—In1—Se1—Cu1^{i}	−68.17 (3)	Se4^{iv}—La2—Se2—La1	134.606 (13)
Se2^{ix}—In1—Se1—Cu1^{i}	−167.44 (3)	Se3^{viii}—La2—Se2—La1	74.59 (3)
Se3^{ix}—In1—Se1—Cu1^{i}	107.42 (3)	Se3^{ix}—La2—Se2—La1	−74.59 (3)
Se3^{viii}—In1—Se1—Cu1^{i}	16.97 (3)	Se3^{x}—La2—Se2—La1	180.0

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*+1/2, *y*, −*z*+3/2; (iv) −*x*+1/2, −*y*, *z*+1/2; (v) −*x*+1/2, −*y*+1, *z*+1/2; (vi) *x*, *y*+1, *z*; (vii) *x*, *y*−1, *z*; (viii) −*x*+1/2, −*y*, *z*−1/2; (ix) −*x*+1/2, −*y*+1, *z*−1/2; (x) *x*−1/2, *y*, −*z*+3/2; (xi) *x*−1/2, *y*, −*z*+1/2; (xii) *x*+1/2, *y*, −*z*+1/2.

Fig. 1

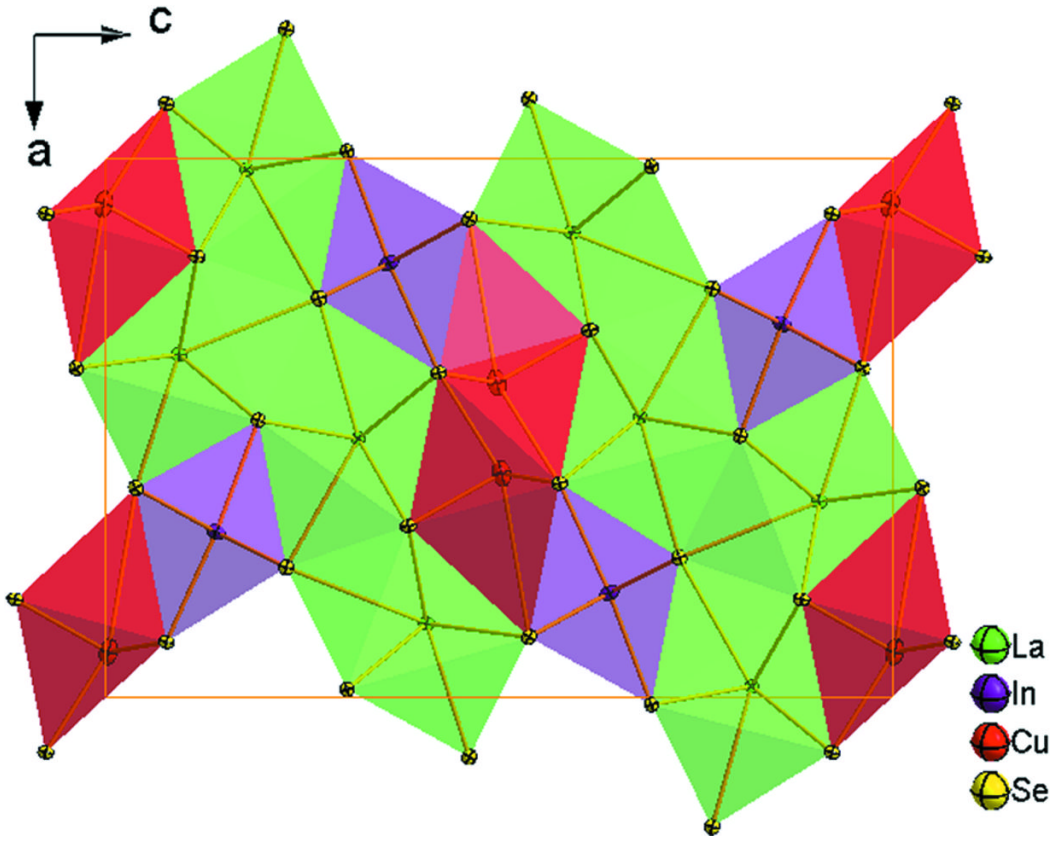
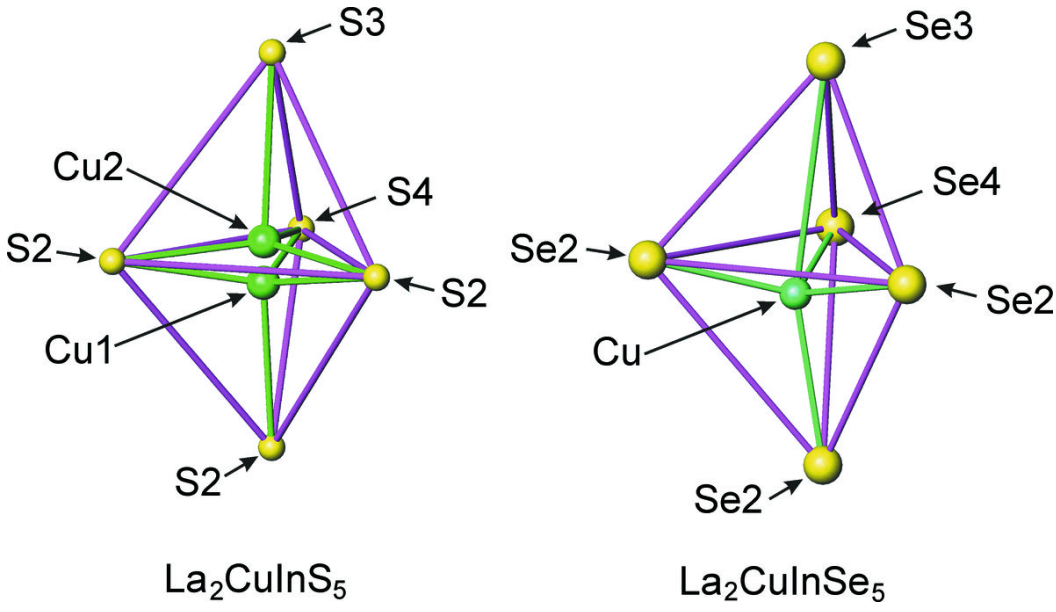


Fig. 2



La_2CuInS_5 $La_2CuInSe_5$