

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rouxelite_full_o

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: rouxelite_full_o

Bond precision:	Cu- S = 0.0106 Å	Wavelength=0.71073
Cell:	a=43.1883 (12) b=8.1037 (2) c=38.147 (1)	
	alpha=96.001 (2) beta=116.615 (2) gamma=95.372 (2)	
Temperature:	295 K	
	Calculated	Reported
Volume	11721.7 (6)	11721.7 (6)
Space group	C -1	C -1
Hall group	-C 1	-C 1
Moiety formula	Ag _{2.10} As _{1.45} Cu ₈ Hg _{3.06} O _{2.52} Pb _{83.55} S _{261.48} Sb _{111.84} Tl ₂	?
Sum formula	Ag _{2.10} As _{1.45} Cu ₈ Hg _{3.06} O _{2.52} Pb _{83.55} S _{261.48} Sb _{111.84} Tl ₂	Ag _{0.50} As _{0.53} Cu ₂ Hg _{0.75} O ₀ Pb _{21.23} S _{65.43} Sb _{27.49} Tl _{10.50}
Mr	41217.98	10317.25
D _x , g cm ⁻³	5.839	5.846
Z	1	4
Mu (mm ⁻¹)	39.590	40.004
F ₀₀₀	17543.9	17558.0
F ₀₀₀ '	17246.12	
h, k, l _{max}	64, 12, 57	64, 12, 57
N _{ref}	41276	55765
T _{min} , T _{max}	0.246, 0.670	0.057, 0.069
T _{min} '	0.087	

Correction method= # Reported T Limits: T_{min}=0.057 T_{max}=0.069
AbsCorr = MULTI-SCAN

Data completeness= 1.351

Theta (max)= 32.173

R(reflections)= 0.0854(17982)

wR2(reflections)=
0.2755(55765)

S = 0.951

Npar= 1131

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.



Alert level B

PLAT213_ALERT_2_B Atom S51 has ADP max/min Ratio 4.2 oblate

Author Response: This is a disordered S atom which we couldn't properly refine as split position.

PLAT213_ALERT_2_B Atom S53 has ADP max/min Ratio 4.2 oblate

Author Response: This is a disordered S atom which we couldn't properly refine as split position.

PLAT213_ALERT_2_B Atom S65 has ADP max/min Ratio 4.2 prolat

Author Response: This is a disordered S atom which we couldn't properly refine as split position.

PLAT213_ALERT_2_B Atom S66 has ADP max/min Ratio 4.2 prolat

Author Response: This is a disordered S atom which we couldn't properly refine as split position.

PLAT213_ALERT_2_B Atom S51' has ADP max/min Ratio 4.2 oblate

Author Response: This is a disordered S atom which we couldn't properly refine as split position.

PLAT213_ALERT_2_B Atom S53' has ADP max/min Ratio 4.2 oblate

Author Response: This is a disordered S atom which we couldn't properly refine as split position.

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note
2 0 0, -4 0 1, -2 0 1, 0 0 1, 2 0 1, -4 0 2,
-2 0 2, 0 0 2, 2 0 2, -2 0 3, 0 0 3,

Author Response: This is a twinned crystal with a huge cell. Integration was difficult with many reflection overlaps. Overall the data set is 99% complete and the data to parameter ratio is excellent.



Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
 _refine_diff_density_min given = -6.381
 Test value = -6.150

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
 The relevant atom site should be identified.

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
 The relevant atom site should be identified.

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 Calc: Ag2.10 As1.45 Cu8 Hg3.06 O2.52 Pb83.55 S261.48
 Sb111.84 Tl2
 Rep.: Ag0.50 As0.53 Cu2 Hg0.75 O0 Pb21.23 S65.43 Sb2
 7.49 Tl0.50

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 51.02 Check

PLAT051_ALERT_1_C Mu(calc) and Mu(cif) Ratio Differs from 1.0 by . 1.04 %

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.28 Report

PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 6.74 eA-3

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -6.38 eA-3

PLAT155_ALERT_4_C The Triclinic Unit Cell is NOT Reduced Please Do !

PLAT220_ALERT_2_C NonSolvent Resd 1 S Ueq(max)/Ueq(min) Range 4.1 Ratio

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S64 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Sb16 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Sb19 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S24 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S42 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S55 Check

PLAT723_ALERT_1_C Torsion Calc 20.00, Rep 23(22) Dev... 3.00 Sigma

SB23-PB28-ME28-S7 1_555 1_555 1_555 4_556 # 344 Check

PLAT723_ALERT_1_C Torsion Calc 136.00, Rep 139(21) Dev... 3.00 Sigma

SB23-PB28-ME28-S37 1_555 1_555 1_555 1_545 # 437 Check

PLAT723_ALERT_1_C Torsion Calc -20.00, Rep -23(22) Dev... 3.00 Sigma

S7 -PB28-ME28-SB23 4_556 1_555 1_555 1_555 # 443 Check

PLAT723_ALERT_1_C Torsion Calc -136.00, Rep -139(21) Dev... 3.00 Sigma

S37 -PB28-ME28-SB23 1_545 1_555 1_555 1_555 # 448 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 9.635 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.526 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 235 Report

31 -1 0, 38 -6 0, 40 -6 0, -40 6 1, -32 2 1, -31 1 1,
 20 0 1, 31 -1 1, 38 -6 1, -40 6 2, -32 0 2, -32 2 2,
 -31 -1 2, -31 1 2, -30 0 2, -28 0 2, 14 4 2, 20 4 2,
 30 -2 2, 30 0 2, -40 6 3, -32 0 3, -32 2 3, -31 -1 3,
 -30 0 3, -28 0 3, -26 0 3, -24 0 3, 12 -4 3, 22 -4 3,
 30 -2 3, -40 6 4, -33 1 4, -32 0 4, -32 2 4, -31 -1 4,
 -30 0 4, -28 0 4, -26 0 4, 16 0 4, 22 0 4, 24 6 4,
 -42 6 5, -34 2 5, -33 1 5, -32 0 5, -31 -1 5, -30 -2 5,
 -30 0 5, -28 0 5, 20 2 5, 24 6 5, 26 6 5, 28 -2 5,
 28 0 5, -42 6 6, -33 1 6, -32 0 6, -31 -1 6, -30 -2 6,

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-30  0  6, -16  0  6, -12  6  6,  4  2  6,  24  6  6,  26  6  6,
 28 -2  6,  30  2  6, -42  6  7, -40  6  7, -33  1  7, -32  0  7,
-31 -1  7, -30 -2  7, -30  0  7, -16  6  7, -14  6  7, -12  6  7,
 22 -2  7,  22  6  7,  24  6  7,  26 -2  7,  26  6  7, -34  0  8,
-33 -1  8, -33  1  8, -32  0  8, -31 -1  8, -30 -2  8,  6 -2  8,
 22  6  8,  26 -2  8,  32 -2  8, -34  0  9, -33 -1  9, -32 -2  9,
PLAT992_ALERT_5_C Repd & Actual _reflns_number_gt Values Differ by      15 Check

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Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and the formula from the _atom_site* data.
 Atom count from _chemical_formula_sum: Ag0.5 As0.53 Cu2 Hg0.75 Pb21.23
 Atom count from the _atom_site data: Ag0.525 As0.363 Cu2 Hg0.764 O0.6

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
 symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 4

From the CIF: _chemical_formula_sum Ag0.50 As0.53 Cu2 Hg0.75 O0 Pb21.2

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Ag	2.00	2.10	-0.10
As	2.12	1.45	0.67
Cu	8.00	8.00	0.00
Hg	3.00	3.06	-0.06
O	4.00	2.52	1.48
Pb	84.92	83.55	1.37
S	261.72	261.48	0.24
Sb	109.96	111.84	-1.88
Tl	2.00	2.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	10	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT017_ALERT_1_G	Check Scattering Type Consistency of ME17	as	PB
PLAT017_ALERT_1_G	Check Scattering Type Consistency of ME18	as	PB
PLAT017_ALERT_1_G	Check Scattering Type Consistency of ME19	as	SB
PLAT017_ALERT_1_G	Check Scattering Type Consistency of ME22	as	SB
PLAT017_ALERT_1_G	Check Scattering Type Consistency of ME27	as	SB
PLAT017_ALERT_1_G	Check Scattering Type Consistency of ME28	as	SB
PLAT017_ALERT_1_G	Check Scattering Type Consistency of ME20	as	SB
PLAT017_ALERT_1_G	Check Scattering Type Consistency of ME21	as	SB
PLAT017_ALERT_1_G	Check Scattering Type Consistency of ME23	as	SB
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C-1	P-1	Note
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	5	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	16	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	4	Report
PLAT299_ALERT_4_G	Atom Site Occupancy Constrained at	0.5	Check
	Pb12 Tl12		
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	14%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	9	Note
	Me17 Me18 Me19 Me22 Me27 Me28 Me20 Me21 Me23		
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb5 (II)	.	1.98 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb7 (II)	.	2.00 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb8 (II)	.	1.96 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Pb9 (II) . 1.81 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Pb10 (II) . 1.82 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Pb11 (II) . 1.96 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Pb13 (II) . 1.88 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Pb14 (II) . 2.06 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Pb15 (II) . 1.82 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Pb16 (II) . 1.79 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb1 (III) . 3.07 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb4 (III) . 3.40 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb5 (III) . 2.99 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb7 (III) . 2.91 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb8 (III) . 2.69 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb10 (III) . 3.18 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb11 (III) . 3.08 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb12 (III) . 2.90 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb13 (III) . 2.45 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb14 (III) . 3.08 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb15 (III) . 2.66 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb17 (III) . 3.18 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb18 (III) . 2.83 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb25 (III) . 2.45 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Sb26 (III) . 2.73 Info
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 8 Note
 PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
 PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
 PLAT908_ALERT_2_G Max. Perc. Data with I > 2*s(I) per Res.Shell . 66.36% Note
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2957 Note
 PLAT931_ALERT_5_G CIFcalcFCF Twin Law (1-2 1) Est.d BASF 0.53 Check
 PLAT931_ALERT_5_G CIFcalcFCF Twin Law [0-1 0] Est.d BASF 0.47 Check
 PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 52 Note
 -38 -2 1, -28 4 2, -26 -2 19, -26 0 4, -24 4 22, -22 0 24,
 -18 -4 1, -18 2 9, -18 2 10, -16 -2 11, -16 -2 12, -16 0 6,
 -16 0 12, -16 0 27, -16 2 10, -14 -2 13, -12 2 15, -12 2 26,
 -10 -2 1, -10 -2 17, -10 -2 28, -10 2 25, -8 -4 1, -8 -2 27,
 -8 4 15, -8 4 16, -6 0 17, -6 0 26, -4 -4 19, -4 -4 20,
 2 0 11, 4 2 6, 6 -2 8, 10 -2 22, 10 0 21, 12 -4 3,
 12 -2 1, 12 0 10, 12 0 14, 14 -4 10, 14 4 2, 16 0 4,
 18 -4 6, 20 0 1, 20 2 5, 20 4 2, 22 -4 3, 22 -2 7,
 22 0 4, 26 0 15,
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.5 Low
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.892 Note
 Predicted wR2: Based on SigI**2 9.53 or SHELX Weight 28.97

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 7 **ALERT level B** = A potentially serious problem, consider carefully
 27 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 58 **ALERT level G** = General information/check it is not something unexpected

24 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 20 ALERT type 2 Indicator that the structure model may be wrong or deficient
 8 ALERT type 3 Indicator that the structure quality may be low
 10 ALERT type 4 Improvement, methodology, query or suggestion
 30 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

Datablock rouxelite_full_o - ellipsoid plot

