

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) new

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: new

Bond precision: La-Rh = 0.0011 A Wavelength=0.71073
Cell: a=16.2667 (5) b=4.5858 (2) c=11.0068 (4)
 alpha=90 beta=90 gamma=90
Temperature: 290 K

	Calculated	Reported
Volume	821.06 (5)	821.06 (5)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	La ₈ Rh _{12.49} Sb ₁₆	La ₂ Rh _{3.122} Sb ₄
Sum formula	La ₈ Rh _{12.49} Sb ₁₆	La ₂ Rh _{3.12} Sb ₄
Mr	4344.79	1086.16
Dx, g cm ⁻³	8.787	8.787
Z	1	4
Mu (mm ⁻¹)	29.103	29.103
F000	1834.1	1834.0
F000'	1809.07	
h, k, lmax	20, 5, 13	20, 5, 13
Nref	917	916
Tmin, Tmax	0.007, 0.030	0.513, 1.000
Tmin'	0.002	

Correction method= # Reported T Limits: Tmin=0.513 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta (max)= 25.999

R(reflections)= 0.0250 (832)

wR2(reflections)=
0.0560 (916)

S = 1.135

Npar= 62

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 C**

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 Rh Ueq(max)/Ueq(min) Range	4.8 Ratio
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.1 Note
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.186 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2 Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.29Ang From Sb2	1.89 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.22Ang From Sb1	1.64 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.68Ang From Sb3	-1.73 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.76Ang From Sb4	-1.66 eA-3

● **Alert level G**

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250 Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.72 Why ?
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem A	88 %Fit
PLAT300_ALERT_4_G	Atom Site Occupancy of Rh4 Constrained at	0.1225 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	2% Note
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	6 Info
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	2 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4 Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	52.0 Degree

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

11 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

9 ALERT type 2 Indicator that the structure model may be wrong or deficient

5 ALERT type 3 Indicator that the structure quality may be low

2 ALERT type 4 Improvement, methodology, query or suggestion

3 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.

