



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision:	O- C = 0.0072 Å	Wavelength=0.41000
Cell:	a=4.4750 (2) alpha=90	b=6.4691 (8) beta=90
Temperature:	293 K	c=9.013 (3) gamma=90
	Calculated	Reported
Volume	260.92 (9)	260.919 (2)
Space group	C m c m	C m c m
Hall group	-C 2c 2	-C -2x; -2yc
Moiety formula	C4 O14 Si2, 2 (Ca)	?
Sum formula	C4 Ca2 O14 Si2	C4 Ca2 O14 Si2
Mr	408.38	408.40
Dx, g cm ⁻³	5.198	5.198
Z	2	2
Mu (mm ⁻¹)	0.626	0.616
F000	408.0	408.0
F000'	408.49	
h, k, lmax	7, 11, 15	5, 11, 12
Nref	404	83
Tmin, Tmax	0.998, 0.999	0.599, 1.000
Tmin'	0.998	

Correction method= # Reported T Limits: Tmin=0.599 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.205

Theta(max)= 20.760

R(reflections)= 0.0437(72)

wR2(reflections)=

wR= 0.0564(83)

S = 2.060

Npar= 16

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 A

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 8.11 Degree

Author Response: Measurement in Diamond anvil cell with 33 degree angle opening

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.650 Why?

Author Response: Measurement in Diamond anvil cell with 33 degree angle opening

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00

Goodness of fit given = 2.060

PLAT088_ALERT_3_C Poor Data / Parameter Ratio 9.44 Note

PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -C -2x;-2y Check

PLAT741_ALERT_1_C Bond Calc 4.4750(15), Rep 4.47500 Missing s.u.

CA1 -CA1 1_555 1_455 # 1 Check

PLAT741_ALERT_1_C Bond Calc 4.4750(15), Rep 4.47500 Missing s.u.

CA1 -CA1 1_555 1_655 # 2 Check

PLAT920_ALERT_1_C Theta(Max) in CIF and FCF Differ by 0.20 Degree

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From Ol . 0.52 eA-3

PLAT992_ALERT_5_C Repd & Actual _reflns_number_gt Values Differ by 48 Check

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !

PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check

PLAT092_ALERT_4_G Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka 0.41000 Ang.

PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 88 Units

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check

PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found Please Check

PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !

PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 3.45 Note

1 1 0, 0 0 2,

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PLAT911_ALERT_3_G Missing FCF Refl Between Thmin & STh/L= 0.600 58 Report
      2 0 0, 4 0 0, 3 1 0, 5 1 0, 2 2 0, 4 2 0,
      3 3 0, 4 4 0, 3 5 0, 3 1 1, 5 1 1, 4 2 1,
      3 3 1, 4 4 1, 3 5 1, 2 0 2, 4 0 2, 3 1 2,
      5 1 2, 4 2 2, 4 4 2, 5 1 3, 0 2 3, 4 2 3,
      4 4 3, 0 6 3, 0 0 4, 4 0 4, 0 2 4, 4 2 4,
      ( 28 More Missing: see the .ckf listing file)
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 136 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 3 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 3 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 1.797 Note
      Predicted wR2: Based on SigI**2 6.90 or SHELX Weight 6.90

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

12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
9 ALERT type 5 Informative message, check

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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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

A reduced cell check using CCDC's cellCheckCSD service has found that one or more structures in this CIF are similar to those previously published in the CSD or the ICSD.

Datablock 1 - ellipsoid plot

