

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: CaSiHx

Bond precision:	Si-Si = 0.0082 A	Wavelength=1.54059	
Cell:	a=14.6356(10)	b=3.81207(15)	c=11.2115(7)
	alpha=90	beta=90	gamma=90
Temperature:	294 K		
	Calculated	Reported	
Volume	625.51(6)	625.51(6)	
Space group	P n m a	Pnma	
Hall group	-P 2ac 2n	-P 2ac 2n	
Moiety formula	H1.60 Si12, 12(Ca H)	?	
Sum formula	Ca12 H13.60 Si12	Ca3 H3.4 Si3	
Mr	831.75	207.94	
Dx,g cm-3	2.208	2.208	
Z	1	4	
Mu (mm-1)	27.377	0.000	
F000	421.6	0.0	
F000'	429.43		
h,k,lmax	14,3,11		
Nref	387		
Tmin,Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.000 Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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

PLAT041_ALERT_1_C	Calc.	and Reported	SumFormula	Strings	Differ	Please Check
PLAT077_ALERT_4_C	Unitcell	Contains	Non-integer	Number of Atoms	..	Please Check
PLAT751_ALERT_4_C	Bond	Calc	1.30000, Rep	1.296(6)	Senseless s.u.
	CA1	-H1	1.555	1.555	# 1 Check
PLAT751_ALERT_4_C	Bond	Calc	2.82000, Rep	2.824(6)	Senseless s.u.
	CA1	-H2	1.555	3.565	# 2 Check
PLAT751_ALERT_4_C	Bond	Calc	2.82000, Rep	2.824(6)	Senseless s.u.
	CA1	-H2	1.555	3.555	# 3 Check
PLAT751_ALERT_4_C	Bond	Calc	2.94000, Rep	2.941(5)	Senseless s.u.
	CA1	-H3	1.555	3.565	# 4 Check
PLAT751_ALERT_4_C	Bond	Calc	2.94000, Rep	2.941(5)	Senseless s.u.
	CA1	-H3	1.555	3.555	# 5 Check
PLAT751_ALERT_4_C	Bond	Calc	1.34000, Rep	1.338(5)	Senseless s.u.
	CA2	-H2	1.555	1.555	# 6 Check
PLAT751_ALERT_4_C	Bond	Calc	2.82000, Rep	2.825(5)	Senseless s.u.
	CA2	-H1	1.555	3.554	# 7 Check
PLAT751_ALERT_4_C	Bond	Calc	2.82000, Rep	2.825(5)	Senseless s.u.
	CA2	-H1	1.555	3.564	# 8 Check
PLAT751_ALERT_4_C	Bond	Calc	3.05000, Rep	3.050(5)	Senseless s.u.
	CA2	-H3	1.555	3.564	# 11 Check
PLAT751_ALERT_4_C	Bond	Calc	3.05000, Rep	3.050(5)	Senseless s.u.
	CA2	-H3	1.555	3.554	# 12 Check
PLAT751_ALERT_4_C	Bond	Calc	1.28000, Rep	1.280(4)	Senseless s.u.
	CA3	-H3	1.555	1.555	# 15 Check
PLAT751_ALERT_4_C	Bond	Calc	3.02000, Rep	3.016(4)	Senseless s.u.
	CA3	-H1	1.555	3.564	# 19 Check
PLAT751_ALERT_4_C	Bond	Calc	3.02000, Rep	3.016(4)	Senseless s.u.
	CA3	-H1	1.555	3.554	# 20 Check
PLAT751_ALERT_4_C	Bond	Calc	3.17000, Rep	3.166(4)	Senseless s.u.
	CA3	-H2	1.555	3.555	# 22 Check
PLAT751_ALERT_4_C	Bond	Calc	3.17000, Rep	3.166(4)	Senseless s.u.
	CA3	-H2	1.555	3.565	# 23 Check
PLAT751_ALERT_4_C	Bond	Calc	2.71000, Rep	2.714(9)	Senseless s.u.
	SI1	-H2	1.555	1.555	# 27 Check
PLAT751_ALERT_4_C	Bond	Calc	3.02000, Rep	3.018(9)	Senseless s.u.
	SI2	-H1	1.555	1.555	# 34 Check
PLAT751_ALERT_4_C	Bond	Calc	1.30000, Rep	1.296(6)	Senseless s.u.
	H1	-CA1	1.555	1.555	# 43 Check
PLAT751_ALERT_4_C	Bond	Calc	2.82000, Rep	2.825(5)	Senseless s.u.
	H1	-CA2	1.555	3.565	# 48 Check
PLAT751_ALERT_4_C	Bond	Calc	2.82000, Rep	2.825(5)	Senseless s.u.
	H1	-CA2	1.555	3.555	# 49 Check
PLAT751_ALERT_4_C	Bond	Calc	3.02000, Rep	3.016(4)	Senseless s.u.
	H1	-CA3	1.555	3.565	# 50 Check
PLAT751_ALERT_4_C	Bond	Calc	3.02000, Rep	3.016(4)	Senseless s.u.
	H1	-CA3	1.555	3.555	# 51 Check
PLAT751_ALERT_4_C	Bond	Calc	3.02000, Rep	3.018(9)	Senseless s.u.
	H1	-SI2	1.555	1.555	# 52 Check
PLAT751_ALERT_4_C	Bond	Calc	1.34000, Rep	1.338(5)	Senseless s.u.
	H2	-CA2	1.555	1.555	# 53 Check
PLAT751_ALERT_4_C	Bond	Calc	2.71000, Rep	2.714(9)	Senseless s.u.
	H2	-SI1	1.555	1.555	# 56 Check
PLAT751_ALERT_4_C	Bond	Calc	2.82000, Rep	2.824(6)	Senseless s.u.
	H2	-CA1	1.555	3.554	# 57 Check
PLAT751_ALERT_4_C	Bond	Calc	2.82000, Rep	2.824(6)	Senseless s.u.
	H2	-CA1	1.555	3.564	# 58 Check
PLAT751_ALERT_4_C	Bond	Calc	3.17000, Rep	3.166(4)	Senseless s.u.
	H2	-CA3	1.555	3.564	# 62 Check
PLAT751_ALERT_4_C	Bond	Calc	3.17000, Rep	3.166(4)	Senseless s.u.
	H2	-CA3	1.555	3.554	# 63 Check

PLAT751_ALERT_4_C Bond	Calc	1.28000, Rep	1.280(4)	Senseless s.u.
H3	-CA3	1.555	1.555	# 64 Check
PLAT751_ALERT_4_C Bond	Calc	2.94000, Rep	2.941(5)	Senseless s.u.
H3	-CA1	1.555	3.564	# 69 Check
PLAT751_ALERT_4_C Bond	Calc	2.94000, Rep	2.941(5)	Senseless s.u.
H3	-CA1	1.555	3.554	# 70 Check
PLAT751_ALERT_4_C Bond	Calc	3.05000, Rep	3.050(5)	Senseless s.u.
H3	-CA2	1.555	3.555	# 71 Check
PLAT751_ALERT_4_C Bond	Calc	3.05000, Rep	3.050(5)	Senseless s.u.
H3	-CA2	1.555	3.565	# 72 Check
PLAT752_ALERT_4_C Angle	Calc	104.00, Rep	104.4(3)	Senseless s.u.
H1	-SI2 -SI3	1.555	1.555 1.555	# 105 Check
PLAT752_ALERT_4_C Angle	Calc	175.00, Rep	175.0(4)	Senseless s.u.
SI2	-H1 -CA1	1.555	1.555 1.555	# 183 Check
PLAT752_ALERT_4_C Angle	Calc	174.00, Rep	174.2(4)	Senseless s.u.
SI1	-H2 -CA2	1.555	1.555 1.555	# 189 Check



Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	1 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...	0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4	Constrained at 0.4 Check

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

2 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
0 **ALERT type 2** Indicator that the structure model may be wrong or deficient
0 **ALERT type 3** Indicator that the structure quality may be low
39 **ALERT type 4** Improvement, methodology, query or suggestion
1 **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.

