



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) yct-byx-ge13

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: yct-byx-ge13

Bond precision: C-C = 0.0026 Å

Wavelength=0.71073

Cell: a=11.7712 (3) b=13.0465 (4) c=14.8559 (4)
 alpha=98.077 (1) beta=107.648 (1) gamma=112.049 (1)
Temperature: 173 K

	Calculated	Reported
Volume	1929.75 (10)	1929.75 (9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C54 H130 Ge2 K2 O4 Si8	C54 H130 Ge2 K2 O4 Si8
Sum formula	C54 H130 Ge2 K2 O4 Si8	C54 H130 Ge2 K2 O4 Si8
Mr	1291.72	1291.67
Dx, g cm ⁻³	1.112	1.111
Z	1	1
Mu (mm ⁻¹)	1.045	1.045
F000	700.0	700.0
F000'	701.48	
h, k, lmax	18, 20, 23	18, 20, 23
Nref	15850	13774
Tmin, Tmax	0.873, 0.901	0.668, 0.747
Tmin'	0.873	

Correction method= # Reported T Limits: Tmin=0.668 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.869

Theta(max)= 34.076

R(reflections)= 0.0377(10943)

wR2(reflections)=
0.0889(13774)

S = 1.054

Npar= 401

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.20	Report
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	4.7	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	5.0	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for Si04 --C19	.	5.8 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for Si05 --C11	.	5.7 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for Si06 --C14	.	5.5 s.u.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of Si05		Check
PLAT751_ALERT_4_C	Bond Calc 3.08000, Rep 3.081(7)		Senseless s.u.
	K1 -H8C 1_555 2_656	#	7 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	27 Report
	1 0 0, -1 1 0, 0 8 0, -8 3 1, 1 -1 2, -8 4 2,		
	2 -2 4, 2 -1 4, 6 -1 4, -6 7 4, 2 -2 5, 3 -2 5,		
	-1 6 5, 1 -8 6, 3 -2 6, 2 -1 6, 3 -6 7, 2 -3 7,		
	2 -2 7, -6 3 8, -5 -2 9, 0 -6 10, -4 -2 10, -2 -1 10,		
	-2 1 10, -3 2 10, 1 -3 11,		
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..		1 Check
	3 0 3,		

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	11	Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H-Atoms	10	Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT189_ALERT_3_G	A Non-default SAME Restraint Value for First Par	0.0100	Report
PLAT189_ALERT_3_G	A Non-default SAME Restraint Value for SecondPar	0.0100	Report
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	20% Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H1AB ..H11B	.	1.94 Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H11B ..H1BD	.	2.02 Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H16C ..H3AC	.	2.12 Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H17A ..H1BC	.	2.14 Ang.
	x,y,z =	1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		11 Note
	Si03 Si04 Si05 Si06 H1AA H1AB H1BC H1BD		
	H3AA H3AB H3AC		
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		142 Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=		2.00 Note

0 1 0, 0 -1 1, 0 0 1,
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2045 Note
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.2 Low
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.168 Note
 Predicted wR2: Based on SigI**2 4.10 or SHELX Weight 8.43
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 10 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 13 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
 5 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. 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

