

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: 3162p21c

Bond precision:	C-C = 0.0193 A	Wavelength=0.71073	
Cell:	a=16.9979(7) alpha=90	b=16.9979(7) beta=90.1(1)	c=43.798(3) gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	12654.5(14)	12654.5(11)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C40 H102 K4 Li4 O12 Si8, C33 H77 K Li4 O10 Si4	C33 H77 K Li4 O10 Si4, C40 H102 K4 Li4 O12 Si8	
Sum formula	C73 H179 K5 Li8 O22 Si12	C73 H179 K5 Li8 O22 Si12	
Mr	1997.27	1997.25	
Dx,g cm-3	1.048	1.048	
Z	4	4	
Mu (mm-1)	0.337	0.337	
F000	4320.0	4320.0	
F000'	4329.36		
h,k,lmax	20,20,52	20,20,52	
Nref	22279	22024	
Tmin,Tmax	0.983,0.983		
Tmin'	0.983		

Correction method= Not given

Data completeness= 0.989 Theta(max)= 25.000

R(reflections)= 0.1012(13638) wR2(reflections)= 0.3110(22024)

S = 1.092 Npar= 1146

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

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.
PLAT183_ALERT_1_A Missing _cell_measurement_reflms_used Value Please Do !
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value Please Do !
PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value Please Do !
PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

Alert level B

SHFSU01_ALERT_2_B The absolute value of parameter shift to su ratio > 0.10
Absolute value of the parameter shift to su ratio given 0.153
Additional refinement cycles may be required.
SYMMS02_ALERT_1_B The unit-cell lengths a and b should not be equal for a
monoclinic cell
Cell 16.9979 16.9979 43.7980
Angles 90.0000 90.1000 90.0000
PLAT080_ALERT_2_B Maximum Shift/Error 0.15 Why ?
PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density 4.91 Report
PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem 4 100 %Fit
PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem c 100 %Fit
PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem c 100 %Fit
PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem c 100 %Fit
PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group P4/ncc Check
PLAT149_ALERT_3_B s.u. on the beta Angle is Too Large 0.10 Degree
PLAT230_ALERT_2_B Hirshfeld Test Diff for 010 --C33 . 7.1 s.u.
PLAT234_ALERT_4_B Large Hirshfeld Difference 05 --C13A 0.30 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference 05 --C16B 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C22 --C23 0.26 Ang.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C59 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C64 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C72 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C18 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C23 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C27 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C30 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C24 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C28 Check
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01925 Ang.
PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C23 - C24 . 1.32 Ang.
PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C25 - C26 . 1.32 Ang.
PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C27 - C28 . 1.30 Ang.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.31 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 1.57 eA-3
PLAT234_ALERT_4_C Large Hirshfeld Difference 05 --C13B 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21 --C22 0.22 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C61 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C62 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C66 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C68 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C70 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C26 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si6 Check

PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	Si8	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	Si9	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	Si10	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	Si12	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C58	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C60	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C63	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C65	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C69	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C71	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C73	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	Si1	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	Si2	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	Si3	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	Si4	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	O5	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	O10	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C17	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C20	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C21	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C25	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C29	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared	to Neighbors	of	C32	Check
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond	C60	-	C61	.	1.42 Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond	C62	-	C63	.	1.41 Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond	C66	-	C67	.	1.41 Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond	C68	-	C69	.	1.41 Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond	C70	-	C71	.	1.40 Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond	C72	-	C73	.	1.42 Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond	C17	-	C18	.	1.36 Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond	C19	-	C20	.	1.41 Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond	C29	-	C30	.	1.35 Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond	C31	-	C32	.	1.37 Ang.

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	19	Report
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.16	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	13.32	Why ?
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	3	Units
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	6	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	6	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13C Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13D Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14A Constrained at	0.5	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H14B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16D	Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		8%	Note
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C40	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C48	Check
PLAT721_ALERT_1_G	Bond Calc 0.96000, Rep 0.97000 Dev...		0.01	Ang.
	C14A -H14B 1.555 1.555	# 147		Check
PLAT721_ALERT_1_G	Bond Calc 0.96000, Rep 0.97000 Dev...		0.01	Ang.
	C13B -H13D 1.555 1.555	# 155		Check
PLAT721_ALERT_1_G	Bond Calc 0.96000, Rep 0.97000 Dev...		0.01	Ang.
	C16B -H16C 1.555 1.555	# 163		Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .		1.32	Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		745	Check
	O11 -SI5 -LI5 1.555 1.555 1.555		29.60	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		746	Check
	O11 -SI5 -LI7 1.555 1.555 1.555		36.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		768	Check
	O12 -SI6 -K2 1.555 1.555 1.555		42.05	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		769	Check
	O12 -SI6 -K5 1.555 1.555 1.555		40.50	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		783	Check
	O13 -SI7 -K2 1.555 1.555 1.555		40.75	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		784	Check
	O13 -SI7 -K5 1.555 1.555 1.555		42.42	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		803	Check
	O14 -SI8 -LI6 1.555 1.555 1.555		29.70	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		804	Check
	O14 -SI8 -LI8 1.555 1.555 1.555		36.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		831	Check
	O15 -SI9 -LI6 1.555 1.555 1.555		36.40	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		832	Check
	O15 -SI9 -LI7 1.555 1.555 1.555		29.30	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		854	Check
	O16 -SI10 -K3 1.555 1.555 1.555		42.19	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		855	Check
	O16 -SI10 -K4 1.555 1.555 1.555		40.38	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		869	Check
	O17 -SI11 -K3 1.555 1.555 1.555		40.53	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		870	Check
	O17 -SI11 -K4 1.555 1.555 1.555		42.27	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		889	Check
	O18 -SI12 -LI5 1.555 1.555 1.555		36.30	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		890	Check
	O18 -SI12 -LI8 1.555 1.555 1.555		29.40	Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		99	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		8	Note

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

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

PLATON version of 30/01/2018; check.def file version of 30/01/2018

