

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ip223

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: ip223

Bond precision:	C-C = 0.0057 A	Wavelength=0.71073	
Cell:	a=11.117(2)	b=36.425(7)	c=13.538(3)
	alpha=90	beta=96.70(3)	gamma=90
Temperature:	153 K		
	Calculated	Reported	
Volume	5444.6(19)	5444.3(19)	
Space group	P 21/n	P2(1)/n	
Hall group	-P 2yn	?	
Moiety formula	C44 H72 Ce Cl2 Li N4 O2 P2 Si4	?	
Sum formula	C44 H72 Ce Cl2 Li N4 O2 P2 Si4	C44 H72 Ce Cl2 Li N4 O2 P2 Si4	
Mr	1081.32	1081.32	
Dx, g cm ⁻³	1.319	1.319	
Z	4	4	
Mu (mm ⁻¹)	1.118	1.118	
F000	2244.0	2244.0	
F000'	2246.76		
h,k,lmax	14,48,18	14,48,18	
Nref	13502	12841	
Tmin,Tmax		0.556,0.563	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.556 Tmax=0.563
AbsCorr = SPHERE

Data completeness= 0.951 Theta(max)= 28.280

R(reflections)= 0.0363(9987) wR2(reflections)= 0.0859(12841)

S = 0.977 Npar= 569

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 B

PLAT029_ALERT_3_B	_diffn_measured_fraction_theta_full	Low	0.951	Note
PLAT412_ALERT_2_B	Short Intra XH3 .. XHn	H8	.. H18E ..	1.74	Ang.

Alert level C

PLAT220_ALERT_2_C	Large Non-Solvent	C	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT241_ALERT_2_C	High		Ueq as Compared to Neighbors for	C42	Check
PLAT242_ALERT_2_C	Low		Ueq as Compared to Neighbors for	Si1	Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance		4.430	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600		604	Report

Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF			Please Do !
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	Si2	-- C17 ..	7.7	su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Ce	-- C11 ..	8.0	su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Ce	-- C12 ..	8.7	su
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =		5	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		80	Check
	C16' -SI2 -C16	1.555	1.555 1.555	34.20	Deg.
PLAT899_ALERT_4_G	SHELXL97	is Deprecated and Succeeded by SHELXL		2014	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Th(Min)	...		2	Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		56	Note

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
3 ALERT type 4 Improvement, methodology, query or suggestion
1 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. 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*, 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 21/04/2015; check.def file version of 09/03/2015

