

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lili2CuLT

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: lili2CuLT

Bond precision: C-C = 0.0030 Å Wavelength=1.54184

Cell: a=8.2094(1) b=18.8517(3) c=28.2049(4)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	4365.02(11)	4365.02(11)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C19 H21 O2 S, F6 P, 0.333(C4 H10 O)	C19 H21 O2 S, F6 P, 0.333(C4 H10 O)
Sum formula	C20.33 H24.33 F6 O2.33 P S	C20.333 H24.333 F6 O2.333 P S
Mr	483.09	483.13
Dx, g cm ⁻³	1.470	1.470
Z	8	8
Mu (mm ⁻¹)	2.638	2.638
F000	2000.0	2012.8
F000'	2012.22	
h, k, lmax	10, 23, 35	10, 23, 35
Nref	4613	4576
Tmin, Tmax	0.827, 0.876	0.857, 1.000
Tmin'	0.517	

Correction method= # Reported T Limits: Tmin=0.857 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.992

Theta(max)= 76.960

R(reflections)= 0.0491(4081)

wR2(reflections)=
0.1238(4576)

S = 1.112

Npar= 403

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

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.2 Ratio
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	P1 Check
PLAT331_ALERT_2_C	Small Aver Phenyl C-C Dist C14A --C19A .	1.36 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.190 Check



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	12 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	25 Report
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT073_ALERT_1_G	H-atoms ref, but _hydrogen_treatment Reported as	constr Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.53 Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	7 Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	2 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	3 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O2 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2A Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2A Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3A Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13A Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14A Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15A Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16A Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17A Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18A Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19A Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13A Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13B Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13C Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15 Constrained at	0.55 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H16	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2A	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3A	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13D	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13E	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13F	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15A	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16A	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17A	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18A	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19A	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3S	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1S	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2S	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4S	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5S	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1SA	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1SB	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1SC	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2SA	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2SB	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4SA	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4SB	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5SA	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5SB	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5SC	Constrained at	0.3333	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	45%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 3)	100%	Note
PLAT398_ALERT_2_G	Deviating C-O-C	Angle From 120 for O2	107.3	Degree
PLAT398_ALERT_2_G	Deviating C-O-C	Angle From 120 for O2A	109.3	Degree
PLAT398_ALERT_2_G	Deviating C-O-C	Angle From 120 for O3S	103.7	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O1 ..C11	3.00	Ang.
		-1/2+x,y,1/2-z =	8_556	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		10	Note
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data			Please Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		16.70	Deg.
	C2A -C1 -C2	1_555 1_555 1_555	#	11 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		17.70	Deg.
	O2A -C4 -O2	1_555 1_555 1_555	#	39 Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group	#	15	Check
PLAT793_ALERT_4_G	Model has Chirality at C2	(Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C3	(Centro SPGR)		R Verify
PLAT793_ALERT_4_G	Model has Chirality at C2A	(Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C3A	(Centro SPGR)		R Verify
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms			! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		245	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		36	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		10	Info
PLAT982_ALERT_1_G	The C-f' =	0.0192 Deviates from IT-value =	0.0181	Check
PLAT982_ALERT_1_G	The F-f' =	0.0754 Deviates from IT-value =	0.0727	Check
PLAT982_ALERT_1_G	The O-f' =	0.0524 Deviates from IT-value =	0.0492	Check
PLAT982_ALERT_1_G	The P-f' =	0.3036 Deviates from IT-value =	0.2955	Check
PLAT982_ALERT_1_G	The S-f' =	0.3354 Deviates from IT-value =	0.3331	Check

PLAT983_ALERT_1_G	The	F-f"=	0.0551	Deviates from	IT-Value =	0.0534	Check
PLAT983_ALERT_1_G	The	O-f"=	0.0338	Deviates from	IT-Value =	0.0322	Check
PLAT983_ALERT_1_G	The	P-f"=	0.4370	Deviates from	IT-Value =	0.4335	Check
PLAT983_ALERT_1_G	The	S-f"=	0.5514	Deviates from	IT-Value =	0.5567	Check

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

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 11 ALERT type 2 Indicator that the structure model may be wrong or deficient
 3 ALERT type 3 Indicator that the structure quality may be low
 74 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.

