

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: ld31

Bond precision: C-C = 0.0033 A Wavelength=0.71073

Cell: a=19.0649(7) b=9.1084(4) c=13.1902(5)
 alpha=90 beta=90 gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	2290.49(16)	2290.49(16)
Space group	P n n a	Pnna
Hall group	-P 2a 2bc	?
Moiety formula	C18 H20 Cs Fe N6 O5 S2	?
Sum formula	C18 H20 Cs Fe N6 O5 S2	C18 H20 Cs Fe N6 O5 S2
Mr	653.28	653.28
Dx,g cm-3	1.895	1.894
Z	4	4
Mu (mm-1)	2.451	2.451
F000	1292.0	1292.0
F000'	1293.28	
h,k,lmax	27,13,18	27,13,18
Nref	3566	3544
Tmin,Tmax	0.863,0.929	0.749,0.930
Tmin'	0.727	

Correction method= # Reported T Limits: Tmin=0.749 Tmax=0.930
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 30.690

R(reflections)= 0.0298(2737) wR2(reflections)= 0.0684(3544)

S = 1.049 Npar= 156

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 G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please	Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4	Report
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3F is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3G is Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1) ..	3	% Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.23	Ratio
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	3	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (III)	2.80	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note

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

1 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
1 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
4 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.

