

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: I

Bond precision:	C-C = 0.0055 A	Wavelength=0.71073	
Cell:	a=19.851(1)	b=11.8071(7)	c=12.8277(7)
	alpha=90	beta=100.699(4)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	2954.3(3)	2954.3(3)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C30 H27 Fe3 P S4	C30 H27 Fe3 P S4	
Sum formula	C30 H27 Fe3 P S4	C30 H27 Fe3 P S4	
Mr	714.28	714.28	
Dx,g cm-3	1.606	1.606	
Z	4	4	
Mu (mm-1)	1.810	1.810	
F000	1456.0	1456.0	
F000'	1462.79		
h,k,lmax	24,14,15	23,14,15	
Nref	5815	5721	
Tmin,Tmax	0.761,0.952	0.660,0.965	
Tmin'	0.688		

Correction method= # Reported T Limits: Tmin=0.660 Tmax=0.965
AbsCorr = MULTI-SCAN

Data completeness= 0.984 Theta(max)= 26.000

R(reflections)= 0.0384(3172) wR2(reflections)= 0.0639(5721)

S = 0.827 Npar= 343

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**

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.138

 **Alert level G**

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12	0.138 Report
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (II) .	2.15 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe2 (II) .	2.19 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe3 (II) .	2.18 Info
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2018 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 0 **ALERT level B** = A potentially serious problem, consider carefully
 - 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 7 **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
 - 2 ALERT type 3 Indicator that the structure quality may be low
 - 1 ALERT type 4 Improvement, methodology, query or suggestion
 - 4 ALERT type 5 Informative message, check
-

checkCIF publication errors

 **Alert level A**

PUBL024_ALERT_1_A The number of authors is greater than 9.
Please specify the role of each of the co-authors
for your paper.

 **Alert level G**

PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

- 1 **ALERT level A** = Data missing that is essential or data in wrong format
 - 1 **ALERT level G** = General alerts. Data that may be required is missing
-

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL024_GLOBAL
;
PROBLEM: The number of authors is greater than 9.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 22/12/2019; check.def file version of 13/12/2019

