

# 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: str0602

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Bond precision:    C-C = 0.0031 Å                      Wavelength=0.71073

Cell:                      a=17.2973(10)              b=15.6070(9)              c=20.9270(12)  
                                alpha=90                      beta=90                      gamma=90

Temperature:              150 K

	Calculated	Reported
Volume	5649.4(6)	5649.4(6)
Space group	P b c a	Pbca
Hall group	-P 2ac 2ab	?
Moiety formula	C29 H21 Fe2 O5 P S2	?
Sum formula	C29 H21 Fe2 O5 P S2	C29 H21 Fe2 O5 P S2
Mr	656.25	656.25
Dx,g cm-3	1.543	1.543
Z	8	8
Mu (mm-1)	1.269	1.269
F000	2672.0	2672.0
F000'	2681.22	
h,k,lmax	23,20,27	22,20,27
Nref	7021	6896
Tmin,Tmax	0.820,0.848	0.734,0.852
Tmin'	0.719	

Correction method= # Reported T Limits: Tmin=0.734 Tmax=0.852  
AbsCorr = MULTI-SCAN

Data completeness= 0.982                      Theta(max)= 28.300

R(reflections)= 0.0378( 5634)              wR2(reflections)= 0.0879( 6896)

S = 1.056                      Npar= 352

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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.

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**Alert level C**

ABSTY02\_ALERT\_1\_C An \_exptl\_absorpt\_correction\_type has been given without  
a literature citation. This should be contained in the  
\_exptl\_absorpt\_process\_details field.  
Absorption correction given as multi-scan

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**Alert level G**

PLAT005\_ALERT\_5\_G No Embedded Refinement Details Found in the CIF Please Do !  
PLAT230\_ALERT\_2\_G Hirshfeld Test Diff for O2 --C2 . 5.1 s.u.  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fe1 --C1 . 8.9 s.u.  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fe1 --C2 . 9.1 s.u.  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fe2 --C3 . 6.2 s.u.  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fe2 --C4 . 8.0 s.u.  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fe2 --C5 . 7.7 s.u.  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 75 Do !  
C2 -FE1 -C1 -O1 -122.00 5.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 76 Do !  
P1 -FE1 -C1 -O1 142.00 5.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 77 Do !  
S1 -FE1 -C1 -O1 -27.00 5.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 78 Do !  
S2 -FE1 -C1 -O1 36.00 5.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 79 Do !  
FE2 -FE1 -C1 -O1 -20.00 5.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 80 Do !  
C1 -FE1 -C2 -O2 124.00 5.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 81 Do !  
P1 -FE1 -C2 -O2 -140.00 5.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 82 Do !  
S1 -FE1 -C2 -O2 -32.00 5.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 83 Do !  
S2 -FE1 -C2 -O2 26.00 5.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 84 Do !  
FE2 -FE1 -C2 -O2 23.00 5.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 85 Do !  
C4 -FE2 -C3 -O3 102.00 9.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 86 Do !  
C5 -FE2 -C3 -O3 -156.00 9.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 87 Do !  
S2 -FE2 -C3 -O3 -48.00 9.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 88 Do !  
S1 -FE2 -C3 -O3 2.00 10.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 89 Do !  
FE1 -FE2 -C3 -O3 6.00 9.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 90 Do !  
C3 -FE2 -C4 -O4 -65.00 4.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 91 Do !  
C5 -FE2 -C4 -O4 -166.00 4.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 92 Do !  
S2 -FE2 -C4 -O4 26.00 4.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 93 Do !  
S1 -FE2 -C4 -O4 96.00 4.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 94 Do !  
FE1 -FE2 -C4 -O4 40.00 4.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 95 Do !  
C3 -FE2 -C5 -O5 -146.00 4.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 96 Do !  
C4 -FE2 -C5 -O5 -51.00 4.00 1.555 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 97 Do !  
S2 -FE2 -C5 -O5 123.00 4.00 1.555 1.555 1.555 1.555

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PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #      98 Do !
      S1 -FE2 -C5 -O5      41.00  4.00  1.555  1.555  1.555  1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #      99 Do !
      FE1 -FE2 -C5 -O5      70.00  4.00  1.555  1.555  1.555  1.555
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2      (II)      .      2.66 Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL      2018 Note

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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
34 ALERT level G = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
26 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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## 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_ABSTY02_str0602
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
# end Validation Reply Form

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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* 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.

