

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: str0604

Bond precision: C-C = 0.0049 A

Wavelength=0.71073

Cell: a=14.310(3) b=16.653(4) c=18.478(4)
 alpha=115.075(3) beta=94.809(4) gamma=99.124(3)
Temperature: 150 K

	Calculated	Reported
Volume	3881.4(15)	3881.2(14)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C40 H30 Fe2 O4 P2 S2, C H2 Cl2	?
Sum formula	C41 H32 Cl2 Fe2 O4 P2 S2	C41 H32 Cl2 Fe2 O4 P2 S2
Mr	897.33	897.33
Dx,g cm-3	1.536	1.536
Z	4	4
Mu (mm-1)	1.117	1.117
F000	1832.0	1832.0
F000'	1838.28	
h,k,lmax	19,22,24	18,21,23
Nref	19375	17593
Tmin,Tmax	0.739,0.915	0.745,0.916
Tmin'	0.724	

Correction method= # Reported T Limits: Tmin=0.745 Tmax=0.916

AbsCorr = MULTI-SCAN

Data completeness= 0.908

Theta(max)= 28.340

R(reflections)= 0.0512(12821)

wR2(reflections)= 0.1484(17593)

S = 1.022

Npar= 955

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

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

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C91 Check

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check

PLAT230_ALERT_2_G Hirshfeld Test Diff for O8 --C8 . 5.5 s.u.

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe2 --C3 . 5.3 s.u.

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe2 --C4 . 6.9 s.u.

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe3 --S4 . 5.0 s.u.

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe3 --C5 . 6.7 s.u.

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe4 --C8 . 7.1 s.u.

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 179 Do !

P1 -FE1 -C1 -O1 -118.00 3.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 180 Do !

P2 -FE1 -C1 -O1 154.00 3.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 181 Do !

S2 -FE1 -C1 -O1 -10.00 3.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 182 Do !

S1 -FE1 -C1 -O1 40.00 3.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 183 Do !

FE2 -FE1 -C1 -O1 44.00 3.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 184 Do !

C4 -FE2 -C2 -O2 -106.00 6.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 185 Do !

C3 -FE2 -C2 -O2 -12.00 6.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 186 Do !

S1 -FE2 -C2 -O2 163.00 6.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 187 Do !

S2 -FE2 -C2 -O2 81.00 6.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 188 Do !

FE1 -FE2 -C2 -O2 113.00 6.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 189 Do !

C4 -FE2 -C3 -O3 7.00 14.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 190 Do !

C2 -FE2 -C3 -O3 -92.00 14.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 191 Do !

S1 -FE2 -C3 -O3 98.00 14.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 192 Do !

S2 -FE2 -C3 -O3 17.00 0.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 193 Do !

FE1 -FE2 -C3 -O3 113.00 14.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 194 Do !

C3 -FE2 -C4 -O4 17.00 0.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 195 Do !

C2 -FE2 -C4 -O4 -85.00 7.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 196 Do !

S1 -FE2 -C4 -O4 21.00 7.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 197 Do !

S2 -FE2 -C4 -O4 70.00 7.00 1.555 1.555 1.555 1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 198 Do !

	FE1 -FE2 -C4 -O4	75.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						199 Do !
	P3 -FE3 -C5 -O5	108.00	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 ... #						200 Do !
	P4 -FE3 -C5 -O5	-164.00	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 ... #						201 Do !
	S4 -FE3 -C5 -O5	-52.00	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 ... #						202 Do !
	S3 -FE3 -C5 -O5	0.00	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 ... #						203 Do !
	FE4 -FE3 -C5 -O5	-54.00	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 ... #						204 Do !
	C8 -FE4 -C6 -O6	71.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						205 Do !
	C7 -FE4 -C6 -O6	-24.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						206 Do !
	S4 -FE4 -C6 -O6	161.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						207 Do !
	S3 -FE4 -C6 -O6	-117.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						208 Do !
	FE3 -FE4 -C6 -O6	-154.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						209 Do !
	C8 -FE4 -C7 -O7	-4.00	21.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						210 Do !
	C6 -FE4 -C7 -O7	93.00	21.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						211 Do !
	S4 -FE4 -C7 -O7	-98.00	21.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						212 Do !
	S3 -FE4 -C7 -O7	17.00	0.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						213 Do !
	FE3 -FE4 -C7 -O7	-110.00	21.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						214 Do !
	C7 -FE4 -C8 -O8	145.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						215 Do !
	C6 -FE4 -C8 -O8	43.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						216 Do !
	S4 -FE4 -C8 -O8	-62.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						217 Do !
	S3 -FE4 -C8 -O8	-114.00	7.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						218 Do !
	FE3 -FE4 -C8 -O8	-115.00	7.00	1.555	1.555	1.555	1.555
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe2 (II)						2.65 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe4 (II)						2.68 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
 2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 51 **ALERT level G** = General information/check it is not something unexpected

2 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
 42 ALERT type 4 Improvement, methodology, query or suggestion
 3 ALERT type 5 Informative message, check

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_str0604
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT244_str0604
;
PROBLEM: Low      'Solvent' Ueq as Compared to Neighbors of      C91 Check
RESPONSE: ...
;
# end Validation Reply Form
```

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.

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