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: FeIIpap-5-NO22_320K

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Bond precision:    C-C = 0.0045 A             Wavelength=0.71073

Cell:            a=23.267(18)     b=8.902(7)             c=11.967(9)
                 alpha=90         beta=114.198(13)       gamma=90
Temperature:     320 K

                 Calculated                  Reported
Volume           2261(3)                     2261(3)
Space group      C 2/c                       C 2/c
Hall group       -C 2yc                      ?
Moiety formula   C24 H16 Fe N6 O6            C24 H16 Fe N6 O6
Sum formula      C24 H16 Fe N6 O6            C24 H16 Fe N6 O6
Mr               540.28                      540.28
Dx,g cm-3        1.587                       1.587
Z                4                           4
Mu (mm-1)        0.723                       0.723
F000             1104.0                      1104.0
F000'            1105.85
h,k,lmax         28,11,14                    28,11,14
Nref             2313                        2292
Tmin,Tmax        0.966,0.993                 0.890,0.993
Tmin'            0.904

Correction method= MULTI-SCAN

Data completeness= 0.991          Theta(max)= 26.400

R(reflections)= 0.0431( 1627)     wR2(reflections)= 0.1130( 2292)

S = 1.016                   Npar= 168
```

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
PLAT241_ALERT_2_C High   Ueq as Compared to Neighbors for .....   O1 Check

Alert level G
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF   Please Do !
PLAT128_ALERT_4_G Alternate Setting for Input Space Group   C2/c   I2/a Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL   2014 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
   3 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 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
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: FeIIpap-5-NO22_100K

Bond precision: C-C = 0.0036 A   Wavelength=0.71073

Cell: a=22.948(2)   b=9.0760(8)   c=11.9420(9)
               alpha=90   beta=119.587(2)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2162.9(3)	2162.9(3)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	?
Moiety formula	C24 H16 Fe N6 O6	C24 H16 Fe N6 O6
Sum formula	C24 H16 Fe N6 O6	C24 H16 Fe N6 O6
Mr	540.28	540.28
Dx,g cm-3	1.659	1.659
Z	4	4
Mu (mm-1)	0.756	0.756
F000	1104.0	1104.0
F000'	1105.85	
h,k,lmax	32,12,17	32,12,17
Nref	3309	3294
Tmin,Tmax	0.956,0.992	0.890,0.993
Tmin'	0.879	

Correction method= MULTI-SCAN

Data completeness= 0.995   Theta(max)= 30.520

R(reflections)= 0.0465(2224)   wR2(reflections)= 0.0961(3294)

S = 1.041   Npar= 168

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

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF   Please Do !
PLAT128_ALERT_4_G Alternate Setting for Input Space Group   C2/c   I2/a Note
PLAT432_ALERT_2_G Short Inter X...Y Contact O2   .. C12   ..   2.97 Ang.
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL   2014 Note

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   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
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   1 ALERT type 5 Informative message, check

Datablock: FeIIqsal-5-NO22_100K

Bond precision: C-C = 0.0081 A   Wavelength=0.71073

Cell: a=19.2422(13)   b=10.4155(9)   c=12.9086(10)
               alpha=90   beta=90   gamma=90
Temperature: 100 K

```
             Calculated                Reported
Volume       2587.1(3)                 2587.1(3)
Space group  P c c a                   P c c a
Hall group   -P 2a 2ac                 ?
Moiety formula  C32 H20 Fe N6 O6       C32 H20 Fe N6 O6
Sum formula  C32 H20 Fe N6 O6          C32 H20 Fe N6 O6
Mr           640.39                    640.39
Dx,g cm-3    1.644                     1.644
Z            4                         4
Mu (mm-1)    0.647                     0.647
F000         1312.0                    1312.0
F000'        1313.92
h,k,lmax     21,11,14                  21,11,14
Nref         1886                      1884
Tmin,Tmax    0.940,0.994               0.876,0.994
Tmin'        0.873


Correction method= MULTI-SCAN


Data completeness= 0.999          Theta(max)= 23.320


R(reflections)= 0.0547( 1295)     wR2(reflections)= 0.1557( 1884)


S = 1.036                    Npar= 204
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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.

🟠 **Alert level B**

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
         Calculated sin(theta_max)/wavelength =   0.5570

> **Author Response: This B-type alert is related to the small size of
> single-crystals systematically isolated with this neutral complex and their
> weak diffracting power at high value of theta angles.**

🟡 **Alert level C**

REFNR01_ALERT_3_C Ratio of reflections to parameters is < 10 for a
         centrosymmetric structure
         sine(theta)/lambda   0.5570
         Proportion of unique data used 1.0000
         Ratio reflections to parameters 9.2353
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
         Rint given   0.120
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ....   9.25 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.0081 Ang.

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL      2014 Note
```

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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*, 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.

PLATON version of 20/08/2014; check.def file version of 18/08/2014