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: mo_d8v3221_0m

```
Bond precision:   C-C = 0.0096 A            Wavelength=0.71073

Cell:          a=12.2969(12)    b=16.1579(15)      c=20.7051(18)
               alpha=90         beta=90            gamma=90
Temperature:   122 K

               Calculated                 Reported
Volume         4113.9(7)                  4113.9(7)
Space group    P 21 21 21                 P 21 21 21
Hall group     P 2ac 2ab                  P 2ac 2ab
Moiety formula C30 H24 F18 Fe O12 Pr      C30 H24 F18 Fe O12 Pr
Sum formula    C30 H24 F18 Fe O12 Pr      C30 H24 F18 Fe O12 Pr
Mr             1115.25                    1115.25
Dx,g cm-3      1.801                      1.801
Z              4                          4
Mu (mm-1)      1.659                      1.659
F000           2188.0                     2188.0
F000'          2190.42
h,k,lmax       16,22,28                   16,22,28
Nref           11057[ 6090]               11046
Tmin,Tmax      0.843,0.877                0.472,0.746
Tmin'          0.840

Correction method= # Reported T Limits: Tmin=0.472 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.81/1.00       Theta(max)= 29.128

R(reflections)= 0.0389( 10406)     wR2(reflections)= 0.1026( 11046)

S = 1.094                  Npar= 567
```

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

```
PLAT213_ALERT_2_C Atom F00Q            has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom F01I            has ADP max/min Ratio .....        3.6 prolat
PLAT213_ALERT_2_C Atom F01O            has ADP max/min Ratio .....        3.8 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference F1      --C01L             0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F2B     --C01L             0.18 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.00963 Ang.
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        1 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......  Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      8.73 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        1 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of   C00U Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of   C014 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of   C01D Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of   C01F Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of   C01L Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of   C01Q Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C017 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........     83 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Pr01      (III)    .    3.50 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe02      (III)    .    3.14 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        6 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
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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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.

PLATON version of 23/04/2018; check.def file version of 23/04/2018

NOMOVE FORCED

Prob = 50
Temp = 122

-7 Y

PLATON-Jul 8 15:05:53 2018 - (70316)

F2B
F010
FOOM
CO1Q
F6
FO1I
F1
CO1L
CO1H
CO1G
CO1F
000I
000D
FOOL
CO1B
COOX
PrO1
FOOF
FOOK
FOOE
FOOG
FOOR
CO18
COOU
FOOH
CO1P
CO13
FOON
CO1D
FO1E
FOOQ
CO12
000A
CO1K
0009
CO1J
000C
000C
FOOJ
0003
CO19
COOV
CO11
CO10
CO1A
CO17
0007
000B
COOO
Fe02
COOZ
0008
0004
0005
COOT
COOP
COOY
CO16
0015
CO15
FOOW

Z -128   mo_d8v3221P 21 21 21   R = 0.04   RES=   0   -39 X