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: stock13

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Bond precision:   C-C = 0.0104 A              Wavelength=0.71073

Cell:             a=11.3421(5)     b=15.3291(7)      c=36.7355(18)
                  alpha=90         beta=90           gamma=90
Temperature:      150 K

                  Calculated                  Reported
Volume            6387.0(5)                   6387.0(5)
Space group       P 21 21 21                  P 21 21 21
Hall group        P 2ac 2ab                   P 2ac 2ab
                  2(C21 H24 Fe N9 P S), 4(B   (C21 H24 Fe N9 P S 2+),
Moiety formula    F4), 3(C2 H3 N)             2(B F4 1-), 1.5(C2 H3 N)
                  C48 H57 B4 F16 Fe2 N21 P2   C24 H28.50 B2 F8 Fe N10.50
Sum formula       S2                          P S
Mr                1513.15                     756.57
Dx,g cm-3         1.574                       1.574
Z                 4                           8
Mu (mm-1)         0.671                       0.671
F000              3080.0                      3080.0
F000'             3086.09
h,k,lmax          13,18,45                    13,18,45
Nref              12542[ 6937]                12295
Tmin,Tmax         0.781,0.897                 0.819,0.921
Tmin'             0.757

Correction method= # Reported T Limits: Tmin=0.819 Tmax=0.921
AbsCorr = ANALYTICAL

Data completeness= 1.77/0.98      Theta(max)= 25.999

R(reflections)= 0.0578( 9499)      wR2(reflections)= 0.1180( 12295)

S = 1.018                   Npar= 932
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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 C

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PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........      7.44 Note
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.01037 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn      H8A    .. H92D    ..      2.04 Ang.
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⚪ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        15 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        15 Report
PLAT012_ALERT_1_G No    _shelx_res_checksum found in CIF ........ Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.50 Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         4 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records         1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         2 Report
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       B10 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       B20 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       B30 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6)..     100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7)..     100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8)..      67 % Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   3.24) in Resd. #         6 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.76) in Resd. #         7 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  S1     .. C30     ..      3.16 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C8     .. C92B    ..      3.18 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C8     .. C91B    ..      3.19 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       253 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        10 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
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  22 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
  12 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 27/03/2017; check.def file version of 24/03/2017