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: cu_24jun19a_0m_a

Bond precision: C-C = 0.0223 A Wavelength=1.54178

Cell: a=21.0539(6) b=34.6467(9) c=42.8754(11)
alpha=90 beta=92.986(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	31232.9(14)	31232.9(14)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C192 H125 Fe2 N20 O13 P5 Pt4, 2(F6 P), C3 H6 N O, 2(C3 H8 N O),	C192 H126 Fe2 N20 O14 P5 Pt4, 2(F6 P), 2(C3 H8 N O), 7(H2 O), C
Sum formula	C201 H162 F12 Fe2 N23 O24 P7 Pt4 [+ solvent]	C201 H162 F12 Fe2 N23 O24 P7 Pt4
Mr	4620.36	4620.38
Dx,g cm-3	0.983	0.983
Z	4	4
Mu (mm-1)	4.767	4.767
F000	9192.0	9192.0
F000'	9142.72	
h,k,lmax	25,41,51	25,41,51
Nref	57437	54335
Tmin,Tmax	0.539,0.564	0.503,0.753
Tmin'	0.489	

Correction method= # Reported T Limits: Tmin=0.503 Tmax=0.753
AbsCorr = NONE

Data completeness= 0.946 Theta(max)= 68.437

R(reflections)= 0.0936(23276)

wR2(reflections)= 0.2715(54335)

S = 0.883 Npar= 2458

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

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low . 0.952 Why?
PLAT260_ALERT_2_B Large Average Ueq of Residue Including P502 0.360 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including P503 0.334 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including O510 0.516 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including O513 0.368 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including O514 0.461 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including O515 0.337 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including O516 0.449 Check
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02225 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C115 - C116 . 1.59 Ang.
PLAT420_ALERT_2_B D-H Bond Without Acceptor O515 --H51A . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O515 --H51B . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O512 --H51C . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O512 --H51D . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O511 --H51E . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O513 --H51G . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O513 --H51H . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O516 --H51I . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O516 --H51J . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O514 --H51K . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O514 --H51L . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O510 --H51M . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O510 --H51N . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O505 --H505 . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O506 --H506 . Please Check
PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ... ! Note

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Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.134
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.134 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 43% Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.27 Report
PLAT213_ALERT_2_C Atom O103 has ADP max/min Ratio ..... 3.1 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference P501 --O501 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P501 --O504 . 0.19 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C104 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C105 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C117 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C211 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C217 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C223 Check

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C227 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C308 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C324 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C339 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C340 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C341 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C342 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C419 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C424 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C440 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C442 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Fe41 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       P101 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       N306 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       N406 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C109 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C133 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C307 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C327 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C338 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       C503 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       N501 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C506 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       N502 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       N503 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    2)        2.3 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    3)        3.3 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pt1      0.104 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O507      0.268 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O508      0.270 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O509      0.201 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O505      0.187 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O511      0.253 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O512      0.211 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O507 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O508 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O509 Check
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C301     - C321     .       1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C309     - C310     .       1.54 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C311     - C327     .       1.54 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C406     - C438     .       1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C411     - C427     .       1.53 Ang.
PLAT415_ALERT_2_C Short Inter D-H..H-X       H51C     ..H244     .       2.11 Ang.
                                                      x,y,z  =      1_555 Check
PLAT415_ALERT_2_C Short Inter D-H..H-X       H51D     ..H323     .       2.04 Ang.
                                                      x,y,z  =      1_555 Check
PLAT415_ALERT_2_C Short Inter D-H..H-X       H51I     ..H236     .       2.01 Ang.
                                     -1/2+x,3/2-y,1/2+z  =      4_576 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         27 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms         273 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............         16 Report
              H506  H505  H51M  H51N  H51E  H51F  H51C  H51D  H51G  H51H  H51K
              H51L  H51A  H51B  H51I  H51J
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PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C192 H125 Fe2 N20 O13 P5 Pt4, 2(F6 P), C3 H6 N O, 2(C3 H8 N
             Rep.: C192 H126 Fe2 N20 O14 P5 Pt4, 2(F6 P), 2(C3 H8
                   N O), 7(H2 O), C3 H6 N O
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.15 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         14 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          3 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       P502 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       P503 Check
PLAT344_ALERT_2_G Unusual sp?       Angle Range in Solvent/Ion for       C506 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C504 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C505 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C507 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C508 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C501 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C502 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe31      (III)     .       2.86 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe41      (III)     .       3.04 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       2582 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         12 Note
              -1  4  3,   1  1  3,  -2  1 10,   3  2  2,   1  5  0,   1  2  1,
              -2  0  4,  -1  5  3,  -1  3  2,   5  0  1,   2  2  8,  -2  2  3,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.2 Low
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
26 **ALERT level B** = A potentially serious problem, consider carefully
61 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
28 **ALERT level G** = General information/check it is not something unexpected

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

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 15/07/2024; check.def file version of 15/07/2024

Datablock cu_24jun19a_0m_a - ellipsoid plot