checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Fe4tponOAc4

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: Fe4tponOAc4

Bond precision: C-C = 0.0057 A Wavelength=0.71075

Cell: a=14.911(9) b=15.8727(10) c=21.010(12)
alpha=103.593(8) beta=98.223(4) gamma=116.470(7)
Temperature: 113 K

	Calculated	Reported
Volume	4148(3)	4147(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C72 H92 Fe4 N12 O10, 4(C24 H20 B), 5(C3 H6 O)	C72 H92 Fe4 N12 O10, 5(C3 H6 O), 4(C24 H20 B)
Sum formula	C183 H202 B4 Fe4 N12 O15	C183 H202 B4 Fe4 N12 O15
Mr	3076.21	3076.19
Dx,g cm-3	1.232	1.232
Z	1	1
Mu (mm-1)	0.408	0.408
F000	1628.0	1628.0
F000'	1629.96	
h,k,lmax	19,20,27	19,20,27
Nref	19022	18858
Tmin,Tmax	0.920,0.972	0.860,1.000
Tmin'	0.846	

Correction method= # Reported T Limits: Tmin=0.860 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 27.481

R(reflections)= 0.0618(12606) wR2(reflections)= 0.1903(18858)

S = 1.075 Npar= 1008

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

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PLAT910_ALERT_3_B Missing FCF Reflection(s) Below Theta(Min)[Deg]=       3.04 Note
                1  0  0,  -2  1  0,  -1  1  0,   0  1  0,   1  1  0,  -1  2  0,
                0 -2  1,   1 -2  1,  -1 -1  1,   0 -1  1,   1 -1  1,  -1  0  1,
                0  0  1,   1  0  1,  -2  1  1,  -1  1  1,   0  1  1,   1 -2  2,
               -1 -1  2,   0 -1  2,   1 -1  2,  -1  0  2,   0  0  2,   1  0  2,
                   (    3 More NOT listed: see .ckf listing file)
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Author Response: The missing reflections at low theta are due to the beamstop shadow/saturation.

Alert level C

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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
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C72 H92 Fe4 N12 O10, 4(C24 H20 B), 5(C3 H6 O)
             Rep.: C72 H92 Fe4 N12 O10, 5(C3 H6 O), 4(C24 H20 B)
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours        C78 Check
PLAT243_ALERT_4_C High MinorResAtom  Ueq as Compared to Neighbours        C91 Check
PLAT244_ALERT_4_C Low  MinorResAtom  Ueq as Compared to Neighbours        C88 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O7      0.124 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O8      0.265 Check
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C91      - C93      .       1.38 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.414 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         52 Report
                4  1  0,   5  1  0,  10  8  0,  -9  4  1,  -3  0  2,  -4  4  2,
                2  3  3,  -7  4  3,   2  9  3,   4-12  5, -12 -6  5, -11 -6  5,
                1  2  5,   7  9  5,  -7 -8  6,   4 -7  6,  -3  4  6,  -6 -2  7,
                0  1  7,  -2  4  7,   9  6  7,   6  9  7,  -7 -2  8,   0  1  8,
               -7  2  8,  -5  2  8,  -8 -8  9,  -8 -7  9,   0  1  9,   7  2  9,
                   (   22 More NOT listed: see .ckf listing file)
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.75Ang From O7      .      -0.55 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.07Ang From O8      .      -0.51 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.87Ang From O8      .      -0.43 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          4 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          4 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.10 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          1 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
              O6      C85     C86     C87     H86A    H86B    H86C    H87A
              H87B    H87C
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    4)        100% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C92 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         10 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit-Cell: Resd.  #          2 Note
              C24 H20 B
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (III)     .       2.99 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2       (III)     .       2.99 Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         44 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         87 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         20 Note
               -9 -6 14,  -8 -8  9,  -8 -7  9,  -8 -4 11,  -8  2 10,  -7 -8  6,
               -7 -1 16,  -7  2  8,  -6  0 16,  -5  2  8,  -5  2 12,  -4  1 18,
               -3  0  2,  -3 13 11,  -2  5 13,  -2  5 15,   0 -1 21,   2  8  9,
                4 -3 21,   4  1  0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.7 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.375 Note
              Predicted wR2: Based on SigI**2  5.64 or SHELX Weight 17.70
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
PLAT994_ALERT_1_G SHELXL .ins Contains no or MERG 0 Instruction ..          ! Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  13 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  25 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  12 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  15 ALERT type 4 Improvement, methodology, query or suggestion
   3 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 15/01/2026; check.def file version of 02/01/2026

duplicate check

No duplication found

Datablock Fe4tponOAc4 - ellipsoid plot

