checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Fe4tponOBz4

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: Fe4tponOBz4

```
Bond precision:   C-C = 0.0063 A          Wavelength=0.71075

Cell:           a=15.827(5)      b=16.106(7)      c=21.217(9)
                alpha=89.47(2)   beta=77.656(19)   gamma=67.251(14)
Temperature:    113 K
```

	Calculated	Reported
Volume	4856(3)	4856(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C92 H100 Fe4 N12 O10, 4(C24 H20 B), 8(C3 H6 O)	C92 H100 Fe4 N12 O10, 8(C3 H6 O), 4(C24 H20 B)
Sum formula	C212 H228 B4 Fe4 N12 O18	C212 H228 B4 Fe4 N12 O18
Mr	3498.70	3498.69
Dx,g cm-3	1.196	1.196
Z	1	1
Mu (mm-1)	0.358	0.358
F000	1852.0	1852.0
F000'	1854.06	
h,k,lmax	20,20,27	20,20,27
Nref	22192	20683
Tmin,Tmax	0.950,0.968	0.872,1.000
Tmin'	0.770	

```
Correction method= # Reported T Limits: Tmin=0.872 Tmax=1.000
AbsCorr = MULTI-SCAN
```

Data completeness= 0.932 Theta(max)= 27.445

R(reflections)= 0.0725(12724) wR2(reflections)= 0.2543(20683)

S = 1.087 Npar= 1173

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

PLAT910_ALERT_3_B Missing FCF Reflection(s) Below Theta(Min)[Deg]= 3.00 Note

1	0	0,	2	0	0,	-1	1	0,	0	1	0,	1	1	0,	2	1	0,
0	2	0,	1	2	0,	-1	-2	1,	0	-2	1,	-1	-1	1,	0	-1	1,
1	-1	1,	-1	0	1,	0	0	1,	1	0	1,	2	0	1,	-1	1	1,
0	1	1,	1	1	1,	2	1	1,	1	2	1,	-1	-1	2,	0	-1	2,

(9 More NOT listed: see .ckf listing file)

Author Response: The missing reflections at low theta are due to the beamstop shadow/saturation.

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Fe1 1.91 eA-3

Author Response: The residual electron densitys near Fe atoms are likely attributed to the inherent limitations in the absorption correction or small systematic errors in the atomic scattering factors for the Fe(III) ions, which are commonly observed in the vicinity of transition metal centers. These peaks do not correspond to any chemically meaningful atoms and do not affect the overall structural model or the validity of the refinement.

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Fe2 1.72 eA-3

Author Response: The residual electron densitys near Fe atoms are likely attributed to the inherent limitations in the absorption correction or small systematic errors in the atomic scattering factors for the Fe(III) ions, which are commonly observed in the vicinity of transition metal centers. These peaks do not correspond to any chemically meaningful atoms and do not affect the overall structural model or the validity of the refinement.

Alert level C

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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.960 Why?

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C92 H100 Fe4 N12 O10, 4(C24 H20 B), 8(C3 H6 O)
             Rep.: C92 H100 Fe4 N12 O10, 8(C3 H6 O), 4(C24 H20 B)
PLAT244_ALERT_4_C Low  MinorResAtom  Ueq as Compared to Neighbours        C98 Check
PLAT244_ALERT_4_C Low  MinorResAtom  Ueq as Compared to Neighbours       C101 Check
PLAT244_ALERT_4_C Low  MinorResAtom  Ueq as Compared to Neighbours       C104 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O6      0.115 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O9      0.116 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O10      0.120 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00628 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.495 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        724 Report
               16  0  0, -11  1  0,   3  1  0,  12  1  0,  16  1  0, -13  2  0,
               -9  2  0,   2  2  0, -13  3  0, -11  3  0,  -9  3  0,  -7  3  0,
              -13  4  0, -10  4  0,  -8  4  0,   1  4  0,  13  4  0, -13  5  0,
               -9  5  0, -10  6  0,  16 11  0,  -3 13  0,   2 14  0,   4 14  0,
               -5 15  0,  -2 15  0,   2 15  0,   3 15  0,   2 16  0,   2 17  0,
                   (  694 More NOT listed: see .ckf listing file)
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          8 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          8 Report
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..       0.73 mm
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.14 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          4 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          2 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          2 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 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      C95     C96     C97     H96A    H96B    H96C    H97A
             H97B    H97C    O10     C107    C108    C109    H10P    H10Q
             H10R    H10S    H10T    H10U
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    4)        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    8)        100% Note
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H10Q     ..H36      .       2.07 Ang.
                                          1-x,1-y,1-z  =      2_666 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H10R     ..H15A     .       1.96 Ang.
                                             x,y,z  =      1_555 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         10 Check
PLAT793_ALERT_4_G Model has Chirality at N3          (Centro SpGr)          S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (III)     .       2.94 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2       (III)     .       2.92 Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         88 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        750 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         13 Note
             -11 -2  6,  -7  8  1,  -3 13  0,  -2  1  2,  -1  2  2,   0 -1  5,
               1  2  5,   1  3  3,   2 -1  1,   2  2  0,   5-11  2,   5-10  3,
              16  6 14,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.283 Note
             Predicted wR2: Based on SigI**2  5.94 or SHELX Weight 23.39
```

```
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
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  29 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
   9 ALERT type 3 Indicator that the structure quality may be low
  17 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. 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 Fe4tponOBz4 - ellipsoid plot

