checkCIF/PLATON report

Structure factors have been supplied for datablock(s) pgo928b_0m

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: pgo928b_0m

Bond precision: C-C = 0.0085 A Wavelength=1.54178

Cell:	a=9.872(11)	b=9.893(9)	c=10.889(13)
	alpha=77.72(4)	beta=84.23(4)	gamma=89.29(3)
Temperature:	293 K		

	Calculated	Reported
Volume	1033.8(19)	1033.8(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H18 Fe2 N2 O15	C18 H18 Fe2 N2 O15
Sum formula	C18 H18 Fe2 N2 O15	C18 H18 Fe2 N2 O15
Mr	614.04	614.04
Dx,g cm-3	1.973	1.973
Z	2	2
Mu (mm-1)	12.098	12.099
F000	624.0	624.0
F000'	621.77	
h,k,lmax	11,11,12	11,11,12
Nref	3521	3409
Tmin,Tmax	0.804,0.834	0.510,0.753
Tmin'	0.136	

Correction method= # Reported T Limits: Tmin=0.510 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.968 Theta(max)= 64.988

R(reflections)= 0.0671(2487) wR2(reflections)= 0.2034(3409)

S = 1.071 Npar= 355

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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THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
          Calculated sin(theta_max)/wavelength =    0.5878
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.968 Why?
PLAT088_ALERT_3_C Poor Data / Parameter Ratio .....................      9.60 Note
PLAT148_ALERT_3_C s.u. on the      a    - Axis is (Too) Large ....      0.011 Ang.
PLAT148_ALERT_3_C s.u. on the      c    - Axis is (Too) Large ....      0.013 Ang.
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.3 Note
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00853 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C9       - C10      .      1.54 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.128 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588       112 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From O13     .      0.47 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.02Ang From O11     .      0.44 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.04Ang From O14     .     -0.46 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.95Ang From O10     .     -0.46 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H1        .     -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H15A      .     -0.31 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         5 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        12 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.13 Report
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.         3 Note
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (II)      .      2.06 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2       (II)      .      2.07 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         2 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       57% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       2.3 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..     130.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
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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
 16 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

  2 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
 11 ALERT type 3 Indicator that the structure quality may be low
  2 ALERT type 4 Improvement, methodology, query or suggestion
  5 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 12/09/2022; check.def file version of 09/08/2022

Datablock pgo928b_0m - ellipsoid plot