

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C16H18N3SFeCN5NO

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: C16H18N3SFeCN5NO

Bond precision:	C-C = 0.0043 A	Wavelength=0.70000
Cell:	a=7.9790(2) b=15.0782(2) c=15.1639(2)	
	alpha=90 beta=100.228(2) gamma=90	
Temperature:	100 K	
	Calculated	Reported
Volume	1795.36(6)	1795.36(6)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C5 Fe N6 O, 2(C16 H18 N3 S)	2(C16 H18 N3 S), C5 Fe N6 O
Sum formula	C37 H36 Fe N12 O S2	C37 H36 Fe N12 O S2
Mr	784.75	784.75
Dx,g cm-3	1.452	1.452
Z	2	2
Mu (mm-1)	0.559	0.565
F000	816.0	816.0
F000'	817.35	
h,k,lmax	10,19,19	10,19,19
Nref	4288	4163
Tmin,Tmax		0.446,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.446 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.971 Theta(max)= 27.420

R(reflections)= 0.0706(3513) wR2(reflections)= 0.2060(4163)

S = 1.040 Npar= 282

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

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.975 Why?

Author Response: The synchrotron measurement conducted consisted in the only full 360 degrees rotation around the spindle axis, thus resulting in a fraction of the reciprocal space left uncollected.

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.3 Note

Author Response: The presence of static displacive disorder affects the U(i,j) components.

PLAT412_ALERT_2_C Short Intra XH3 .. XHn H2A ..H4 . 1.89 Ang.
x,y,z = 1_555 Check

Author Response: The methyl-aromatic CH distance is a result of the geometry of the molecule. CH3 orientation was refined and converged to the reported value. This may be due to the presence of static disorder.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 4.173 Check

Author Response: The presence of static displacive disorder negatively influences the value at issue.

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 80 Report

Author Response: The synchrotron measurement conducted consisted in the only full 360 degrees rotation around the spindle axis, thus resulting in a fraction of the reciprocal space left uncollected.



Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 8 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.70000 Ang.
PLAT153_ALERT_1_G The s.u.'s on the Cell Axes are Equal ..(Note) 0.0002 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 12 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 10 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 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 4 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe1 --C19 . 17.7 s.u.

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1	--N8	.	21.3 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of N4		Constrained at		0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N6		Constrained at		0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1		Constrained at		0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2		Constrained at		0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17		Constrained at		0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19		Constrained at		0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N7		Constrained at		0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N8		Constrained at		0.25 Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)			62% Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact	N6	..C16		2.90 Ang.
			x,y,z =	1_555	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				180 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			45 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF				1 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...				29 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				1 Info
PLAT984_ALERT_1_G	The Fe-f' =	0.3555	Deviates from the B&C-Value		0.3456 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 33 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 ALERT type 3 Indicator that the structure quality may be low
 17 ALERT type 4 Improvement, methodology, query or suggestion
 0 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 22/04/2020; check.def file version of 09/03/2020

