

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C16H18N3S3FeCN6xH2O

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: C16H18N3S3FeCN6xH2O

Bond precision:	C-C = 0.0058 A	Wavelength=0.70000
Cell:	a=10.8838(4) b=15.2399(5) c=15.4106(6)	
	alpha=90 beta=102.913(4) gamma=90	
Temperature:	100 K	
	Calculated	Reported
Volume	2491.48(16)	2491.48(16)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C16 H18 N4 S2, 2(C6 Fe N6), 4(C16 H18 N3 S), 2(C8 H9 N), 2(H2 O)	C6 Fe N6, 2(C16 H18 N3 S), 0.5(C16 H18 N4 S2), C8 H9 N, H2 O
Sum formula	C108 H112 Fe2 N30 O2 S6	C54 H56 Fe N15 O S3
Mr	2166.34	1083.16
Dx, g cm ⁻³	1.444	1.444
Z	1	2
Mu (mm ⁻¹)	0.464	0.469
F000	1134.0	1134.0
F000'	1135.67	
h,k,lmax	14,20,20	14,20,20
Nref	5943	5924
Tmin,Tmax		0.324,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.324 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 27.421

R(reflections)= 0.0790(4670) wR2(reflections)= 0.2146(5924)

S = 1.056 Npar= 456

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

PLAT234_ALERT_4_C Large Hirshfeld Difference N4 --C15 . 0.16 Ang.

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

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 negatively influences the value at issue.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 6.903 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 18 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	28	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	9	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.92	Why ?
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.70000	Ang.
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	10	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	14	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	3	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	3	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	4	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of S1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N8A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C26A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C27A	Constrained at	0.5 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H22A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N5	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N5A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N7	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N7A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N8B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C26B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C27B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26F	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27F	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1E	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		62%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 5)		1.50	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H15C ..H26F .		2.07	Ang.
	-1/2+x,1/2-y,1/2+z =		4_566	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .		1.14	Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #		109	Check
	C21A -C20A -S1 1.555 1.555 3.655		30.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #		112	Check
	S1 -C20A -N1 1.555 1.555 3.655		7.80	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #		131	Check
	S1 -C21A -N1 3.655 1.555 1.555		10.70	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #		174	Check
	C21A -S1 -C20A 3.655 1.555 3.655		34.20	Deg.
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ...		!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		135	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		16	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		1	Info
PLAT984_ALERT_1_G	The Fe-f' = 0.3560 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
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
79 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
67 ALERT type 4 Improvement, methodology, query or suggestion
1 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

