checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 321_a

Bond precision: C-C = 0.0058 A Wavelength=0.71073

Cell: a=8.8010(4) b=11.4073(6) c=11.5391(4)
alpha=94.090(2) beta=107.393(1) gamma=100.823(2)
Temperature: 193 K

	Calculated	Reported
Volume	1075.76(8)	1075.76(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C14 H16 Cl2 Fe N6, 2(C H4 O), Cl	C14 H16 Cl2 Fe N6, Cl, 2(C H4 O)
Sum formula	C16 H24 Cl3 Fe N6 O2	C16 H24 Cl3 Fe N6 O2
Mr	494.61	494.61
Dx,g cm-3	1.527	1.527
Z	2	2
Mu (mm-1)	1.098	1.098
F000	510.0	510.0
F000'	511.70	
h,k,lmax	10,13,13	10,13,13
Nref	3797	3780
Tmin,Tmax	0.858,0.877	
Tmin'	0.858	

Correction method= Not given

Data completeness= 0.996 Theta(max)= 24.995

R(reflections)= 0.0467(3134) wR2(reflections)= 0.1284(3780)

S = 1.096 Npar= 257

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

PLAT420_ALERT_2_B D-H Bond Without Acceptor O00S --H00W . Please Check

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Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C14 H16 Cl2 Fe N6, 2(C H4 O), Cl
Rep.: C14 H16 Cl2 Fe N6, Cl, 2(C H4 O)
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H00E ..H00T . 2.12 Ang.
1-x,1-y,1-z = 2_666 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H00I ..H00V . 2.00 Ang.
x,-1+y,z = 1_545 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H00K ..H00V . 2.12 Ang.
x,-1+y,z = 1_545 Check

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report
H008 H00B H00J H00W
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl04 ..C00O . 3.15 Ang.
x,y,z = 1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 52 Note

Fe01	Cl02	Cl03	Cl04	N005	N006	N007	N008
H008	N009	O00A	H00J	N00B	H00B	C00C	C00D
C00E	H00A	H00C	C00F	H00D	H00E	C00G	C00H
H00H	C00I	H00I	C00J	H00F	H00G	C00K	H00K
C00L	H00L	C00M	H00M	C00N	H00N	C00O	H00T
H00U	H00V	C00P	H00P	C00Q	H00Q	C00R	H00O
H00R	H00S	O00S	H00W				

PLAT794_ALERT_5_G Tentative Bond Valency for Fe01 (III) . 2.84 Info
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.2 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree

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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
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 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. 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 13/05/2024; check.def file version of 04/05/2024

Datablock 321_a - ellipsoid plot