checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2870_twin1_hklf4

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: 2870_twin1_hklf4

Bond precision: C-C = 0.0096 A Wavelength=0.71073

Cell: a=14.182(1) b=16.7847(11) c=21.5947(15)
alpha=77.232(6) beta=83.623(6) gamma=89.793(6)
Temperature: 173 K

	Calculated	Reported
Volume	4981.1(6)	4981.1(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C25 H26 Fe N O Si, 3(C25 H28 Fe N O Si), 2(Cl4 Zn)	0.25(C50 H52 Cl4 Fe2 N2 O2 Si2 Zn), 0.25(Cl4 Zn), 0.25(C25 H26
Sum formula	C100 H110 Cl8 Fe4 N4 O4 Si4 Zn2	C25 H27.50 Cl2 Fe N O Si Zn0.50
Mr	2182.06	545.50
Dx,g cm-3	1.455	1.452
Z	2	8
Mu (mm-1)	1.356	1.353
F000	2252.0	2252.0
F000’	2259.42	
h,k,lmax	17,20,26	17,20,26
Nref	19589	22949
Tmin,Tmax	0.771,0.763	0.958,1.000
Tmin’	0.755	

Correction method= # Reported T Limits: Tmin=0.958 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.172 Theta(max)= 26.000

R(reflections)= 0.0520(14671) wR2(reflections)= 0.0945(22949)

S = 0.898 Npar= 1165

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 A

PLAT213_ALERT_2_A Atom C29 has ADP max/min Ratio ..... 9.6 prolat
PLAT213_ALERT_2_A Atom C38A has ADP max/min Ratio ..... 5.9 oblate
PLAT901_ALERT_1_A Cell Parameters in CIF and FCF do not Match .... ! Error

Alert level B

PLAT220_ALERT_2_B Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 6.9 Ratio
PLAT420_ALERT_2_B D-H Without Acceptor O2 -- H2 ... Please Check
PLAT420_ALERT_2_B D-H Without Acceptor O3 -- H3A ... Please Check

Alert level C

PLAT213_ALERT_2_C Atom C33 has ADP max/min Ratio ..... 3.4 oblate
PLAT213_ALERT_2_C Atom C48 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C37A has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C3 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom C6 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C8 has ADP max/min Ratio ..... 3.2 oblate
PLAT213_ALERT_2_C Atom C58 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C68 has ADP max/min Ratio ..... 3.8 oblate
PLAT213_ALERT_2_C Atom C76 has ADP max/min Ratio ..... 3.7 oblate
PLAT213_ALERT_2_C Atom C91 has ADP max/min Ratio ..... 3.2 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 6.0 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 3 C Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 4 C Ueq(max)/Ueq(min) Range 4.4 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 5.8 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 2 H Uiso(max)/Uiso(min) Range 5.1 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C8 -- C9 .. 6.0 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2 -- C37A .. 0.24 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0096 Ang.
PLAT701_ALERT_1_C Bond Calc 2.2352(17), Rep 2.2380(17), Dev.. 1.65 Sigma
ZN1 -CL3 1.555 1.555 ..... # 3 Check
PLAT701_ALERT_1_C Bond Calc 2.2366(17), Rep 2.2394(17), Dev.. 1.65 Sigma
ZN2 -CL8 1.555 1.555 ..... # 11 Check
PLAT702_ALERT_1_C Angle Calc 103.84(6), Rep 103.77(6), Dev.. 1.17 Sigma
CL7 -ZN2 -CL5 1.555 1.555 1.555 .... # 11 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C25 H26 Fe N O Si

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C25 H27.5 Cl2 Fe1 N1 O1 Si1
Atom count from _chemical_formula_moiety:C18.75 H19.5 Cl2 Fe0.75 N0.
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 15 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-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 ... 0.25 Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.006 Degree

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PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1    --  C9      ..        6.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe3    --  C59     ..        6.0 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..          7 % Note
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C36    Check
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C27    -   C36    ..       1.50 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   CL3    --  N1      ..       5.81 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         74 Check
              C11  -N1   -CL3     1.555   1.555   1.555             44.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        436 Check
              CL4  -N3   -H3B     1.555   1.555   1.555             18.20 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
              C25 H28 Fe N O Si
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
              C25 H28 Fe N O Si
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
              C25 H28 Fe N O Si
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
              Cl4 Zn
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
              Cl4 Zn
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1     (II)    .....       1.99 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         48 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          4 Note
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3 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
25 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
25 **ALERT level G** = General information/check it is not something unexpected

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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT213_2870_twin1_hklf4
;
PROBLEM: Atom C29             has ADP max/min Ratio .....        9.6 prolat
RESPONSE: ...
;
_vrf_PLAT901_2870_twin1_hklf4
;
PROBLEM: Cell Parameters in CIF and FCF do not Match ....          ! Error
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 24/11/2016; check.def file version of 23/11/2016

Datablock 2870_twin1_hklf4 - ellipsoid plot