checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0433_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: mo_b0433_0m

Bond precision: C-C = 0.0050 A Wavelength=0.71073

Cell: a=13.9663(10) b=15.8280(11) c=18.8751(13)
alpha=90 beta=105.280(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	4025.0(5)	4025.0(5)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C30 H44 Cl2 Fe2 N2 O2 Si2 Zn2, 0.824(C4 H10 O), 0.176(C3 H6 O)	C30 H44 Cl2 Fe2 N2 O2 Si2 Zn2, 0.82(C4 H10 O), 0.18(C3 H6 O)
Sum formula	C33.82 H53.29 Cl2 Fe2 N2 O3 Si2 Zn2	C33.82 H53.30 Cl2 Fe2 N2 O3 Si2 Zn2
Mr	905.52	905.47
Dx,g cm-3	1.494	1.494
Z	4	4
Mu (mm-1)	2.110	2.110
F000	1872.9	1873.0
F000’	1880.18	
h,k,lmax	18,20,24	18,20,24
Nref	19441[10068]	19405
Tmin,Tmax	0.592,0.852	0.051,0.090
Tmin’	0.269	

Correction method= # Reported T Limits: Tmin=0.051 Tmax=0.090
AbsCorr = MULTI-SCAN

Data completeness= 1.93/1.00 Theta(max)= 27.999

R(reflections)= 0.0217(18722) wR2(reflections)= 0.0538(19405)

S = 1.028 Npar= 906

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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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range        3.9 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C8 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Fe1 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         O5 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min)          9 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         11 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....         7 Note
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Alert level G

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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:   C33.82 H53.3 Cl2 Fe2 N2 O3
           Atom count from _chemical_formula_moiety:C33.82 H53.28 Cl2 Fe2 N2 O3
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....       0.62 mm
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =          48 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   9.70) in Resd. #          4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   3.53) in Resd. #          5 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
             C4 H10 O
PLAT933_ALERT_2_G Number of OMIT records in Embedded RES .....          6 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density           4 Note
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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
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   3 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
   3 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 08/07/2016; check.def file version of 05/07/2016

Datablock mo_b0433_0m - ellipsoid plot