checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0437_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_b0437_0m

Bond precision: C-C = 0.0114 A Wavelength=0.71073

Cell: a=7.841(2) b=32.342(9) c=22.860(6)
alpha=90 beta=90.347(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	5797(3)	5797(3)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C30 H44 Cl2 Fe2 N2 O2 Si2 Zn2, C3 H6 O	C30 H44 Cl2 Fe2 N2 O2 Si2 Zn2, C3 H6 O
Sum formula	C33 H50 Cl2 Fe2 N2 O3 Si2 Zn2	C33 H50 Cl2 Fe2 N2 O3 Si2 Zn2
Mr	892.31	892.27
Dx,g cm-3	1.534	1.534
Z	6	6
Mu (mm-1)	2.197	2.197
F000	2760.0	2760.0
F000’	2770.85	
h,k,lmax	10,43,30	10,43,30
Nref	30272[15394]	29898
Tmin,Tmax	0.778,0.896	0.050,0.083
Tmin’	0.601	

Correction method= # Reported T Limits: Tmin=0.050 Tmax=0.083
AbsCorr = MULTI-SCAN

Data completeness= 1.94/0.99 Theta(max)= 28.795

R(reflections)= 0.0419(26679) wR2(reflections)= 0.0991(29898)

S = 1.110 Npar= 1289

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

PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 2 Check
PLAT939_ALERT_3_B Large Value of Not (SHELXL) Weight Optimized S . 224.04

Alert level C

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01144 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min) 6 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 32 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check

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Alert level G

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 4 Report
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage = 33 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (6.16) in Resd. # 6 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (3.84) in Resd. # 7 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3 Note
C30 H44 Cl2 Fe2 N2 O2 Si2 Zn2
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 79 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT931_ALERT_5_G Found Twin Law ( )[0 0 1] Estimated BASF 0.20 Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
4 **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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
7 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 08/07/2016; check.def file version of 05/07/2016

Datablock mo_b0437_0m - ellipsoid plot

