

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mm019

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: mm019

Bond precision:	C-C = 0.0105 Å	Wavelength=1.54184
Cell:	a=32.3755 (6) alpha=90	b=32.3755 (6) beta=90
		c=32.3755 (6) gamma=90
Temperature:	170 K	
	Calculated	Reported
Volume	33935.1 (19)	33935.2 (18)
Space group	F m -3 m	F m -3 m
Hall group	-F 4 2 3	-F 4 2 3
Moiety formula	C216 N48 O64 Zr12 [+ solvent]	C108 N24 O32 Zr6
Sum formula	C216 N48 O64 Zr12 [+ solvent]	C108 N24 O32 Zr6
Mr	5385.28	2692.64
Dx, g cm-3	0.527	0.527
Z	2	4
Mu (mm-1)	1.714	1.714
F000	5248.0	5248.0
F000'	5259.32	
h, k, lmax	40, 40, 40	26, 34, 38
Nref	1774	1668
Tmin, Tmax	0.855, 0.885	0.886, 0.908
Tmin'	0.845	

Correction method= # Reported T Limits: Tmin=0.886 Tmax=0.908

AbsCorr = ANALYTICAL

Data completeness= 0.940

Theta(max)= 74.645

R(reflections)= 0.0591(1342)

wR2(reflections)=
0.1718(1668)

S = 1.101

Npar= 54

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

PLAT250_ALERT_2_A Large U3/U1 Ratio for Average U(i,j) Tensor 9.1 Note

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.19 Report
PLAT213_ALERT_2_C Atom N2 has ADP max/min Ratio 3.6 prolat
PLAT213_ALERT_2_C Atom C1 has ADP max/min Ratio 3.3 prolat
PLAT213_ALERT_2_C Atom C2 has ADP max/min Ratio 3.5 prolat
PLAT213_ALERT_2_C Atom C3 has ADP max/min Ratio 3.5 prolat
PLAT213_ALERT_2_C Atom C4 has ADP max/min Ratio 3.7 prolat
PLAT213_ALERT_2_C Atom C5 has ADP max/min Ratio 3.6 prolat
PLAT213_ALERT_2_C Atom C6 has ADP max/min Ratio 3.2 prolat
PLAT215_ALERT_3_C Disordered N1 has ADP max/min Ratio 3.4 Note
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Zr1 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Zr1 0.242 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.0105 Ang.
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.339 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 22 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 4 Check
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Zr1 1.03 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.44Ang From O1 . 0.40 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.47Ang From C6 . -0.48 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 8 Report
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 6 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0010 Report
PLAT300_ALERT_4_G Atom Site Occupancy of N1 Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 11% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 1) 127.50 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact N2 ..C6 . 2.55 Ang.
1/2-x,1/2-y,z = 74_555 Check

PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure	!	Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zr1 (IV) .	4.31	Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints	109	Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed	!	Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	65	Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ	14	Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ	6	Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.	2	Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.	2	Units

1 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 19 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 27 **ALERT level G** = General information/check it is not something unexpected

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

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# start Validation Reply Form
vrf PLAT250 mm019
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;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....      9.1 Note
RESPONSE: ...
;
# end Validation Reply Form

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PLATON version of 10/05/2023; check.def file version of 10/05/2023

Datablock mm019 - ellipsoid plot