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: I

Bond precision: C-C = 0.0084 A Wavelength=0.41328

Cell: a=33.6644(6) b=33.6644(6) c=33.6644(6)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	38152(2)	38151.6(12)
Space group	F m -3 m	Fm-3m
Hall group	-F 4 2 3	?
Moiety formula	C54 H24 O16 Zr3	C108 H48 O32 Zr6
Sum formula	C54 H24 O16 Zr3	C108 H48 O32 Zr6
Mr	1202.39	2404.78
Dx,g cm-3	0.419	0.419
Z	8	4
Mu (mm-1)	0.246	0.548
F000	4768.0	4768.0
F000'	4771.05	
h,k,lmax	39,39,39	39,38,36
Nref	1613	1591
Tmin,Tmax		0.947,0.947
Tmin'		

Correction method= MULTI-SCAN

Data completeness= 0.986 Theta(max)= 13.900

R(reflections)= 0.0879(1191) wR2(reflections)= 0.2378(1591)

S = 1.063 Npar= Npar = 25

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

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PLAT230_ALERT_2_B Hirshfeld Test Diff for    O2     --  C1      ..       22.4 su
PLAT241_ALERT_2_B High      Ueq as Compared to Neighbors for .....         C1 Check
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....         O2 Check
PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor ....        6.3 Note
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Alert level C

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THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5813
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        Zr1 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0084 Ang.
PLAT373_ALERT_2_C Long   C(sp)-C(sp)   Bond  C7     -   C7_f   ...       1.39 Ang.
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          6 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension .......          3 Info
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ............       2.00 Ratio
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.18 Why ?
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          8 Units
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .      30114 A**3
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         43 Do !
            C4  -C5  -C6  -C7    180.00  0.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         44 Do !
            C4  -C5  -C6  -C7      0.00  0.00  46.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         45 Do !
            C5  -C6  -C7  -C7      0.00  0.00   1.555   1.555   1.555 121.555
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.47 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Zr1     (IV)    .....       4.11 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         17 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed            ! Info
PLAT952_ALERT_5_G Reported and Calculated Lmax Values Differ by ..          3 Check
PLAT984_ALERT_1_G The  C-f'=     0.002 Deviates from the B&C-Value      0.000
PLAT984_ALERT_1_G The  O-f'=     0.006 Deviates from the B&C-Value      0.002
PLAT984_ALERT_1_G The Zr-f'=    -0.536 Deviates from the B&C-Value      0.163
PLAT985_ALERT_1_G The Zr-f"=     2.614 Deviates from the B&C-Value      1.575
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  22 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   4 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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock I - ellipsoid plot