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: p180811c

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Bond precision:  C-C = 0.0110 A          Wavelength=0.71073

Cell:            a=43.0260(4)     b=43.0260(4)     c=43.0260(4)
                 alpha=90         beta=90          gamma=90
Temperature:     120 K
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	Calculated	Reported
Volume	79651(2)	79651.3(12)
Space group	F m -3 m	F m -3 m
Hall group	-F 4 2 3	?
Moiety formula	C144 H120 N12 O40 Zr12, 6(Cl) [+ solvent]	?
Sum formula	C144 H120 Cl6 N12 O40 Zr12 [+ solvent]	C143.99 H119.99 Cl6 N12 O40 Zr12
Mr	3965.86	3965.54
Dx,g cm-3	0.661	0.661
Z	8	8
Mu (mm-1)	0.371	0.371
F000	15760.0	15760.0
F000’	15485.49	
h,k,lmax	51,51,51	51,51,51
Nref	3437	3432
Tmin,Tmax		
Tmin’		

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Correction method= Not given

Data completeness= 0.999          Theta(max)= 25.000

R(reflections)= 0.0850( 2351)     wR2(reflections)= 0.2810( 3432)

S = 1.084                 Npar= 127
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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

PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ... ! Note

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Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.28 Report
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Zr1 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.011 Ang.

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C143.9899 H119.99 Cl6 N12 O40 Zr
Atom count from the _atom_site data: C144 H120 Cl6 N12 O40 Zr12
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
From the CIF: _cell_formula_units_Z 8
From the CIF: _chemical_formula_sum C143.99 H119.99 Cl6 N12 O40 Zr12
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	1151.92	1152.00	-0.08
H	959.92	960.00	-0.08
Cl	48.00	48.00	0.00
N	96.00	96.00	0.00
O	320.00	320.00	0.00
Zr	96.00	96.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 9 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 509.43 Why ?
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 8 Units
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3 Note
PLAT300_ALERT_4_G Atom Site Occupancy of C6 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2B Constrained at 0.25 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 29% Note

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PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  2          0.25 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .        1.30 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #          85 Check
              C9   -C5   -C6      1.555   1.555   1.555             27.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #          88 Check
              C9   -C5   -C6    187.000   1.555 187.000             27.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #          95 Check
              C7   -C8   -C10   187.000   1.555 187.000             25.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #          98 Check
              C7   -C8   -C10     1.555   1.555   1.555             25.80 Deg.
PLAT794_ALERT_5_G Tentative Bond Valency for Zr1       (IV)      .        4.17 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          61 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed            ! Info
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL        2018 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  36 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
   4 ALERT type 3 Indicator that the structure quality may be low
  22 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 03/05/2019; check.def file version of 29/04/2019

Datablock p180811c - ellipsoid plot