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: MUF-92-15h-77pc

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Bond precision:  O- C = 0.0001 A         Wavelength=0.71075

Cell:           a=17.1440(18)    b=17.1440(18)    c=17.1440(18)
                alpha=90         beta=90          gamma=90
Temperature:    100 K
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	Calculated	Reported
Volume	5038.9(16)	5038.9(16)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	2(C7 H3.50 N0.50 O1.08 Zn0.33), 4(C1.35 H1.16 N0.10 O0.42 Zn0.1	1(C84 H48 N6 O13 Zn4), 1(C32.42 H27.78 N2.32 O10.04 Zn3.09)
Sum formula	C19.40 H12.64 N1.38 O3.84 Zn1.18	C116.41 H75.77 N8.32 O23.04 Zn7.09
Mr	403.85	2423.07
Dx,g cm-3	0.799	0.799
Z	6	1
Mu (mm-1)	0.870	0.870
F000	1229.4	1230.0
F000’	1231.92	
h,k,lmax	15,15,15	15,15,15
Nref	793[450]	795
Tmin,Tmax		0.591,0.746
Tmin’		

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Correction method= # Reported T Limits: Tmin=0.591 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.77/1.00      Theta(max)= 18.812

R(reflections)= 0.1278( 709)      wR2(reflections)= 0.3424( 795)

S = 1.677                 Npar= 66
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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 A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4537
PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 1548 Ang**3

Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.7985 Check
PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing). C8A Check
PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
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
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT082_ALERT_2_C High R1 Value ..... 0.13 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.34 Report
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 6.82 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.19 Report
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . ZN2A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C5A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C6A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C7A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C8A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . N9A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C11A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C12A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C17A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C16A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C15A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C14A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C13A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . N9B Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . ZN2A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C5A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C6A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C7A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C8A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . N9A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C11A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C12A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C17A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C16A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C15A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C14A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C13A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . N9B Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . ZN2A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C5A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C6A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C7A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C8A Check

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PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        N9A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .       C11A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .       C12A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .       C17A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .       C16A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .       C15A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .       C14A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .       C13A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        N9B Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Zn2A      0.172 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Zn2B      0.198 Check
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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:   C116.41 H75.77 N8.32 O23.04 Z
           Atom count from _chemical_formula_moiety:C116.42 H75.78 N8.32 O23.04 Z
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:C116.41 H75.77 N8.32 O23.04 Zn7.
           Atom count from the _atom_site data:  C107.4154 H69.63043 N7.151428 O2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    1
          From the CIF: _chemical_formula_sum  C116.41 H75.77 N8.32 O23.04 Zn7.09
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         116.42    107.42    9.00
          H          75.78     69.64    6.14
          N           8.32      7.15    1.17
          O          23.04     23.04    0.01
          Zn          7.09      3.75    3.34
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         15 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         17 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          3 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     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 ...       6.00 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         12 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          5 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          3 Note
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Zn2A       Constrained at     0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N9A        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5A        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8A        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13A       Constrained at       0.25 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C14A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7A        Constrained at       0.25 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        81% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          3 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #        24 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       120 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
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  2 ALERT level A = Most likely a serious problem - resolve or explain
  3 ALERT level B = A potentially serious problem, consider carefully
 53 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 47 ALERT level G = General information/check it is not something unexpected

 14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 ALERT type 3 Indicator that the structure quality may be low
 73 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 07/08/2019; check.def file version of 30/07/2019

Datablock MUF-92-15h-77pc - ellipsoid plot