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-93-48h-51pc

Bond precision: C-C = 0.0040 A Wavelength=0.71092

Cell: a=17.09(4) b=17.09(4) c=17.09(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	4991(35)	4991(39)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	0.347(C10.50 H6 Co O3.25), 2(C3.50 H O1.08 Zn0.33), 4(C1.75 H1.	1(C84 H48 N6 O13 Zn4), 1(C21.65 H12.37 Co2.06 O6.7)
Sum formula	C17.64 H10.08 Co0.35 N O3.29 Zn0.67	C105.63 H60.37 Co2.06 N6 O19.70 Zn4
Mr	352.74	2111.55
Dx,g cm-3	0.704	0.703
Z	6	1
Mu (mm-1)	0.677	0.675
F000	1071.8	1069.0
F000’	1074.03	
h,k,lmax	13,13,13	13,13,13
Nref	499[289]	494
Tmin,Tmax		0.563,0.746
Tmin’		

Correction method= # Reported T Limits: Tmin=0.563 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.71/0.99 Theta(max)= 15.831

R(reflections)= 0.2048(247) wR2(reflections)= 0.5257(494)

S = 1.915 Npar= 55

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 =    0.3837
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ..................       0.53 Report
PLAT234_ALERT_4_A Large Hirshfeld Difference Zn1      --O2       .       0.35 Ang.
PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of .       1611 Ang**3
```

Alert level B

```
PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 .........     0.7040 Check
PLAT082_ALERT_2_B High R1 Value ..................................       0.20 Report
PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18) ........       5.25 Note
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including       Co2      0.363 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including       Zn1      0.422 Check
PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing).       C15 Check
PLAT987_ALERT_1_B The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
```

Alert level C

```
RADNW01_ALERT_1_C  The radiation wavelength lies outside the expected range
          for the supplied radiation type. Expected range 0.71065-0.71075
          Wavelength given =    0.71092
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
          Rint given   0.173
STRVA01_ALERT_4_C           Flack test results are ambiguous.
         From the CIF: _refine_ls_abs_structure_Flack    0.690
         From the CIF: _refine_ls_abs_structure_Flack_su    0.040
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .........      0.173 Report
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       0.82 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
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..     Please Check
PLAT148_ALERT_3_C s.u. on the      a    - Axis is (Too) Large ....      0.040 Ang.
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .        C12 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .        C13 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .         N1 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .        C15 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .        C16 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .        C17 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .        C18 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .        C19 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .        C20 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .        C21 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C12 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C13 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .         N1 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C15 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C16 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C17 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C18 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C19 Check
```

```
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C20 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C21 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C12 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C13 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .         N1 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C15 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C16 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C17 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C18 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C19 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C20 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C21 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? .       0.69 Check
```

Alert level G

```
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:   C105.6299 H60.37 Co2.06 N6 O1
           Atom count from _chemical_formula_moiety:C105.65 H60.37 Co2.06 N6 O19.
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:C105.6299 H60.37 Co2.06 N6 O19.7
           Atom count from the _atom_site data:  C105.8315 H60.47516 Co2.079833 N
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    1
          From the CIF: _chemical_formula_sum  C105.63 H60.37 Co2.06 N6 O19.70 Zn
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        105.64    105.84   -0.20
          H         60.37     60.48   -0.11
          Co         2.06      2.08   -0.02
          N          6.00      6.00    0.00
          O         19.70     19.76   -0.06
          Zn         4.00      4.00    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 ...         16 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
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
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...         -4 Units
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         11 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          3 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C12       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17       Constrained at       0.25 Check
```

```
PLAT300_ALERT_4_G Atom Site Occupancy of H18        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1         Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13        Constrained at       0.25 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        39% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C14      - C14_b    .       1.50 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..N1               2.52 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..N1               2.52 Ang.
                                                      y,x,z  =     20_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..N1               2.52 Ang.
                                                    1-x,1-y,z  =      3_665 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..N1               2.52 Ang.
                                                    1-y,1-x,z  =     19_665 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..N1               3.00 Ang.
                                                    1-y,x,2-z  =      4_657 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..N1               3.00 Ang.
                                                    y,1-x,2-z  =      2_567 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..N1               3.00 Ang.
                                                    1-x,y,2-z  =      9_657 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..N1               3.00 Ang.
                                                    x,1-y,2-z  =      6_567 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..C15              3.17 Ang.
                                                    1-x,1-y,z  =      3_665 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..C15              3.17 Ang.
                                                    1-y,1-x,z  =     19_665 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..C15              3.17 Ang.
                                                      y,x,z  =     20_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..C15              3.17 Ang.
                                                      x,y,z  =      1_555 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         36 Check
             C12  -C11  -C12    20.555   1.555   1.555             21.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         40 Check
             C12  -C11  -C12    19.665   1.555   3.665             21.30 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         17 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .       2.17 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        223 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
```

---

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

17 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
24 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
60 ALERT type 4 Improvement, methodology, query or suggestion
3 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 07/08/2019; check.def file version of 30/07/2019

Datablock MUF-93-48h-51pc - ellipsoid plot