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: xt8018-c-1-13

Bond precision: C-C = 0.0329 A Wavelength=0.02510

Cell: a=22.461(5) b=22.461(5) c=22.461(5)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	11332(8)	11331(8)
Space group	P m -3 n	P m -3 n
Hall group	-P 4n 2 3	-P 4n 2 3
Moiety formula	C98 H38 Cl12 N54 Zn15 [+ solvent]	C98 H38 Cl12 N54 Zn15, 12[CH4O]
Sum formula	C98 H38 Cl12 N54 Zn15 [+ solvent]	C110 H86 Cl12 N54 O12 Zn15
Mr	3378.07	3762.55
Dx,g cm-3	0.990	1.103
Z	2	2
Mu (mm-1)	0.000	0.000
F000	0.0	1228.0
F000'	3314.83	
h,k,lmax	18,18,18	18,18,18
Nref	653	652
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.998 Theta(max)= 0.599

R(reflections)= 0.1230(287) wR2(reflections)= 0.4373(652)

S = 1.049 Npar= 79

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

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.880

Author Response: Powder crystal collected by Micro-ED

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4165

Author Response: The diffraction of powder crystal was weak at high angles.

PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 ..... 0.880 Report

Author Response: Powder crystal collected by Micro-ED

Alert level B

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.44 Report
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.03286 Ang.

Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 44% Check
PLAT082_ALERT_2_C High R1 Value ..... 0.12 Report
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 8.27 Note
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C005 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Zn1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N004 Check

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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:C110 H86 Cl12 N54 O12 Zn15
Atom count from the _atom_site data: C98 H38 Cl12 N54 Zn15

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
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    2
           From the CIF: _chemical_formula_sum  C110 H86 Cl12 N54 O12 Zn15
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        220.00    196.00   24.00
           H        172.00     76.00   96.00
           Cl        24.00     24.00    0.00
           N        108.00    108.00    0.00
           O         24.00      0.00   24.00
           Zn        30.00     30.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
              Calc: C98 H38 Cl12 N54 Zn15
              Rep.: C110 H86 Cl12 N54 O12 Zn15
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
              Calc: C98 H38 Cl12 N54 Zn15
              Rep.: C98 H38 Cl12 N54 Zn15, 12[CH4O]
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.16 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      14.97 Why ?
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 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
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C005     ..C00D     .       2.49 Ang.
                                       -1/2+z,1/2-y,1/2+x  =     22_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C005     ..C005     .       2.87 Ang.
                                        1/2-y,1/2-x,3/2-z  =     14_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C005     ..C005     .       2.98 Ang.
                                       1/2-x,-1/2+z,1/2+y  =     18_545 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C00D     ..C00D     .       2.58 Ang.
                                       -1/2+z,1/2-y,1/2+x  =     22_455 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in  Crystal Structure          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          15 Note
              Zn00    Cl00    N004    C005    N006    C007    N008    C009
              H009    C00A    N00B    C00C    H00C    C00D    H00D
PLAT768_ALERT_4_G RES Embedded Explicitly Supplied Scattering Data          6 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .       1.82 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn00      (II)      .       2.06 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............         87 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT948_ALERT_5_G Externally Supplied Scattering Factors       RES          6 Note
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3 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
6 **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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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 11 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT084_xt8018-c-1-13
;
PROBLEM: High wR2 Value (i.e. > 0.25) ...................       0.44 Report
RESPONSE: ...
;
_vrf_PLAT341_xt8018-c-1-13
;
PROBLEM: Low Bond Precision on  C-C Bonds ...............    0.03286 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 17/09/2025; check.def file version of 17/09/2025

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duplicate check

No duplication found

Datablock xt8018-c-1-13 - ellipsoid plot