

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-93-72h-62pc

Bond precision: C-C = 0.0040 Å

Wavelength=0.71092

Cell: a=17.06(4) b=17.06(4) c=17.06(4)
 alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	4965(35)	4970(38)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	0.413(C10.50 H6 Co 03.25), 2(C3.50 H 01.08 Zn0.33), 4(C1.75 H1.	1(C84 H48 N6 O13 Zn4), 1(C25.84 H14.77 Co2.46 O8)
Sum formula	C18.34 H10.48 Co0.41 N 03.51 Zn0.67	C109.80 H62.74 Co2.46 N6 020.99 Zn4
Mr	368.95	2208.24
Dx, g cm-3	0.740	0.738
Z	6	1
Mu (mm-1)	0.715	0.712
F000	1120.6	1118.0
F000'	1123.00	
h, k, lmax	13, 13, 13	13, 13, 13
Nref	553[319]	551
Tmin, Tmax		0.583, 0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.583 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.73/1.00 Theta(max)= 16.504

R(reflections)= 0.1699(393) wR2(reflections)= 0.3848(551)

S = 1.513 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 $\sin(\theta_{\max})/\lambda$ is less than 0.550

Calculated $\sin(\theta_{\max})/\lambda = 0.3996$

PLAT601_ALERT_2_A Structure Contains Solvent Accessible Voids of . 1592 Ang**3

Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm⁻³ 0.7400 Check
PLAT082_ALERT_2_B High R1 Value 0.17 Report
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.38 Report
PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18) 5.80 Note
PLAT260_ALERT_2_B Large Average Ueq of Residue Including Co2 0.319 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including Zn1 0.306 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 0.140

STRVA01_ALERT_4_C Flack test results are ambiguous.

From the CIF: _refine_ls_abs_structure_Flack 0.610

From the CIF: _refine_ls_abs_structure_Flack_su 0.040

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.140 Report
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.978 Why?
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 0.91 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
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C10 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	02 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? .	0.61 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: C109.8 H62.74 Co2.46 N6 O20.9
 Atom count from _chemical_formula_moiety: C109.84 H62.77 Co2.46 N6 O21

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: C109.8 H62.74 Co2.46 N6 O20.99 Z
 Atom count from the _atom_site data: C110.0311 H62.87496 Co2.479801 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 C109.80 H62.74 Co2.46 N6 O20.99 Zn
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	109.81	110.04	-0.23
H	62.75	62.88	-0.13
Co	2.46	2.48	-0.02
N	6.00	6.00	0.00
O	20.99	21.06	-0.07
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 ... -3 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 2 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
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.
	x,y,z =	1_555		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.
	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 ..N1		3.00	Ang.
	1-y,x,2-z =	4_657		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.
	1-x,1-y,z =	3_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		21.26	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) .		2.19	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 !	
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		3	Note

2 **ALERT level A** = Most likely a serious problem - resolve or explain
 8 **ALERT level B** = A potentially serious problem, consider carefully
 47 **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
 26 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 59 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.

