



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: nu6000-nahco3-2_auto

Bond precision:	C-C = 0.0139 Å	Wavelength=0.02510
Cell:	a=22.134 (3)	b=22.134 (3)
	alpha=90	beta=90
Temperature:	293 K	c=22.134 (3)
		gamma=90
	Calculated	Reported
Volume	10844 (4)	10843 (4)
Space group	P m -3 n	P m -3 n
Hall group	-P 4n 2 3	-P 4n 2 3
Moiety formula	2(C15.57 H5 N9 O3.14 Zn2.50) [+ solvent]	C93.429 H30 N54 O18.857 Zn15, 32[CH4O]
Sum formula	C31.14 H10 N18 O6.29 Zn5 solvent]	[+ C125.44 H158 N54 O50.88 Zn15]
Mr	1063.86	4217.24
Dx, g cm ⁻³	0.978	1.292
Z	6	2
Mu (mm ⁻¹)	0.000	0.000
F000	0.0	1419.0
F000'	3137.81	
h, k, lmax	23,23,23	23,22,23
Nref	1186	1187
Tmin, Tmax		0.432, 1.000
Tmin'		

```
Correction method= # Reported T Limits: Tmin=0.432 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.001          Theta (max) = 0.749
R(reflections) = 0.1360( 769)          wR2 (reflections) =
S = 1.263          Npar= 98
0.3725( 1187)
```

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 0.519

Author Response: The data set was collected by electron diffraction. The relatively high Rint value is due to the weak diffraction and limited resolution due to the small crystal size.

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5208

Author Response: The data set was collected by electron diffraction. The relatively low sine(theta_max)/wavelength is due to the weak diffraction and limited resolution due to the small crystal size.

PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 0.519 Report

Author Response: The data set was collected by electron diffraction. The relatively high Rint value is due to the weak diffraction and limited resolution due to the small crystal size.

Alert level B

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.37 Report

Author Response: The data set was collected by electron diffraction. The relatively high wR2 value is due to the weak diffraction and limited resolution due to the small crystal size.

🟡 Alert level C

PLAT082_ALERT_2_C High R1 Value 0.14 Report
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.01386 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H4 ..H4 1.90 Ang.
-1/2+y, 1/2+x, 3/2-z = 13_456 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: C125.44 H158 N54 O50.88 Zn15
Atom count from _chemical_formula_moiety: C125.4290 H158 N54 O50.85699
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: C125.44 H158 N54 O50.88 Zn15
Atom count from the _atom_site data: C93.43200 H30 N54 O18.864 Zn15
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 C125.44 H158 N54 O50.88 Zn15
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif	sites	diff
C	250.88	186.86	64.02	
H	316.00	60.00	256.00	
N	108.00	108.00	0.00	
O	101.76	37.73	64.03	
Zn	30.00	30.00	0.00	

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 4 Report
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: C31.14 H10 N18 O6.29 Zn5
Rep.: C125.44 H158 N54 O50.88 Zn15
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: 2(C15.57 H5 N9 O3.14 Zn2.50)
Rep.: C93.429 H30 N54 O18.857 Zn15, 32[CH4O]
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 3 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
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 0.0001 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0001 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 16% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact C1 ..C1 . 2.76 Ang.
1-x, 2-y, 1-z = 25_676 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C2 ..C2 . 2.51 Ang.
1-z, 1-x, y = 7_665 Check

PLAT432_ALERT_2_G	Short Inter X...Y Contact	C2 ..C2 .	2.89	Ang.
		-1/2+z, 3/2-y, 1/2+x =	22_465	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Crystal Structure			! Info
PLAT768_ALERT_4_G	RES Embedded Explicitly Supplied Scattering Data			5 Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		0.00	Deg.
	ZN1 -N2 -ZN1 27_575 1_555 1_555	#	33	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		0.00	Deg.
	ZN1 -N3 -ZN1 27_575 1_555 1_555	#	39	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		0.00	Deg.
	ZN1 -O1 -ZN1 27_575 1_555 1_555	#	63	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		0.00	Deg.
	C6 -C6 -O2 27_575 1_555 1_555	#	64	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		0.00	Deg.
	C6 -C6 -O3 27_575 1_555 1_555	#	65	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		0.00	Deg.
	C6 -O2 -C6 27_575 1_555 1_555	#	68	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		0.00	Deg.
	ZN1 -O3 -ZN1 1_555 1_555 27_575	#	69	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		0.00	Deg.
	C6 -O3 -C6 27_575 1_555 1_555	#	72	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn2 (II) .		1.69	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		127	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed			! Info
PLAT948_ALERT_5_G	Externally Supplied Scattering Factors	RES	5	Note
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		1.5	Degree

3 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 39 **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
 9 ALERT type 3 Indicator that the structure quality may be low
 16 ALERT type 4 Improvement, methodology, query or suggestion
 4 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

duplicate check

No duplication found

Datablock nu6000-nahco3-2_auto - ellipsoid plot

