checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2

Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell: a=10.1082(6) b=14.1898(10) c=10.7272(7)
alpha=90 beta=116.467(2) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	1377.38(16)	1377.37(16)
Space group	P 21/n	P21/n
Hall group	-P 2yn	?
Moiety formula	4(C12 H10 Cu N8 O), H2 O	?
Sum formula	C48 H42 Cu4 N32 O5	C12 H10.50 Cu N8 O1.25
Mr	1401.34	350.32
Dx,g cm-3	1.689	1.689
Z	1	4
Mu (mm-1)	1.604	1.604
F000	710.0	710.0
F000'	711.43	
h,k,lmax	12,17,13	12,17,13
Nref	2711	2708
Tmin,Tmax	0.698,0.761	0.709,0.772
Tmin'	0.685	

Correction method= # Reported T Limits: Tmin=0.709 Tmax=0.772
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.990

R(reflections)= 0.0275(2327) wR2(reflections)= 0.0735(2708)

S = 1.051 Npar= 215

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 G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.25 Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1 -- N5_a ..	8.2 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of O2 is Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2A is Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2B is Constrained at	0.25 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)..	100 % Note
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	33 Do !
	CU1 -N6 -N7 -N8 -175.00 4.00 1.555 1.555 1.555 1.555	
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	11 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
2 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

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Publication of your CIF in other journals

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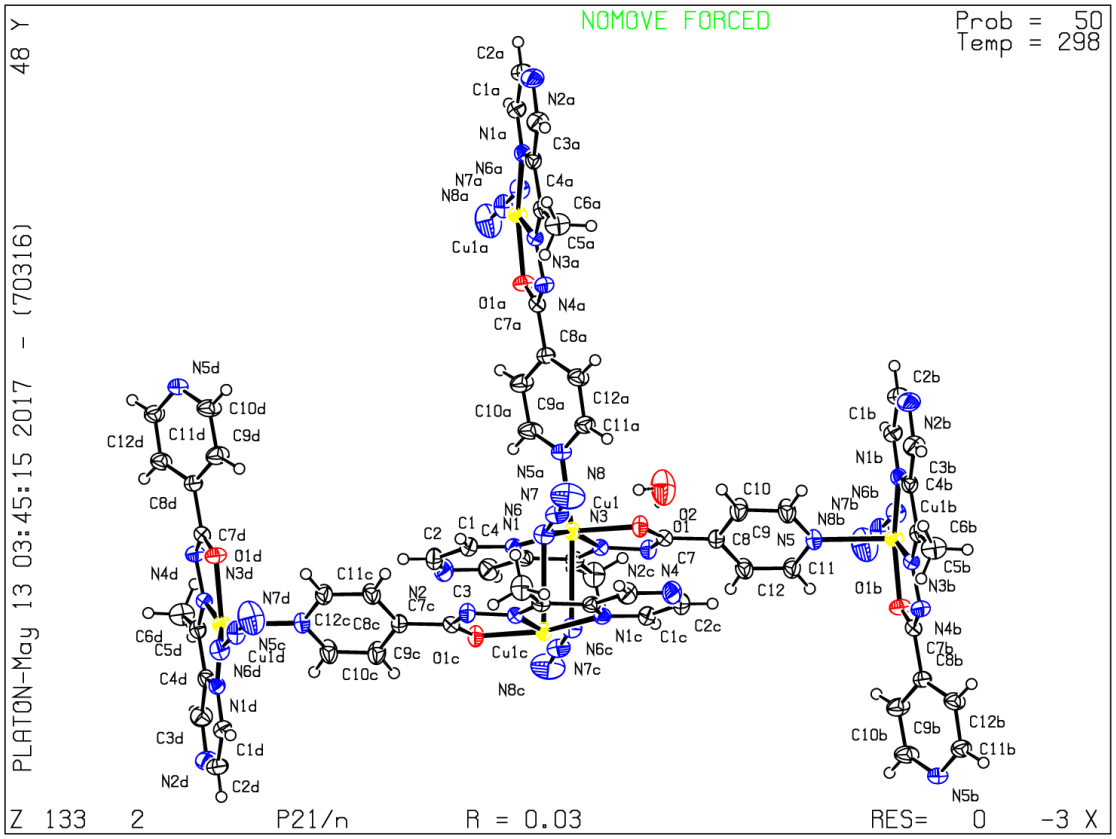
PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock 2 - ellipsoid plot



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3

Bond precision: C-C = 0.0032 A Wavelength=0.71073

Cell: a=10.247(3) b=14.165(4) c=10.703(3)
alpha=90 beta=115.063(8) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	1407.3(7)	1407.3(7)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	2(C12 H10 N8 O Zn), H2 O	?
Sum formula	C24 H22 N16 O3 Zn2	C12 H11 N8 O1.50 Zn
Mr	713.36	356.66
Dx,g cm-3	1.684	1.683
Z	2	4
Mu (mm-1)	1.765	1.765
F000	724.0	724.0
F000'	725.30	
h,k,lmax	12,17,13	12,17,13
Nref	2763	2760
Tmin,Tmax	0.673,0.741	0.687,0.753
Tmin'	0.660	

Correction method= # Reported T Limits: Tmin=0.687 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.000

R(reflections)= 0.0281(2309) wR2(reflections)= 0.0737(2760)

S = 1.059 Npar= 215

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 G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50 Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Zn1 -- N3 ..	5.7 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Zn1 -- N5_a ..	8.2 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of O2 is Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2A is Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2B is Constrained at	0.5 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)..	100 % Note
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	33 Do !
	ZN1 -N6 -N7 -N8 -175.00 4.00 1.555 1.555 1.555 1.555	
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	10 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

```
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```

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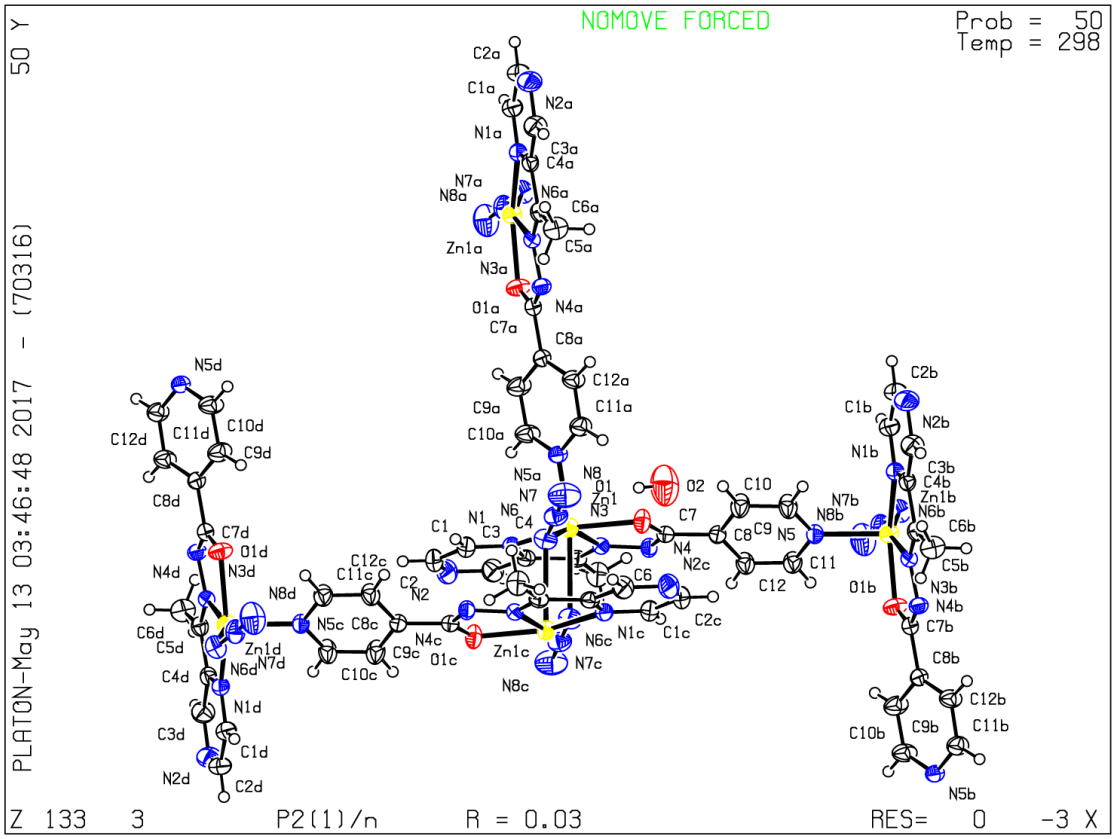
Datablock 3 - ellipsoid plot



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1

```
Bond precision:  C-C = 0.0069 A          Wavelength=0.71073

Cell:          a=10.3084(18)     b=11.1749(19)    c=14.372(2)
               alpha=88.687(5)   beta=89.140(5)   gamma=68.924(5)
Temperature:   298 K
```

	Calculated	Reported
Volume	1544.4(4)	1544.4(5)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C24 H22 Cd2 N16 O3	?
Sum formula	C24 H22 Cd2 N16 O3	C24 H22 Cd2 N16 O3
Mr	807.40	807.38
Dx,g cm-3	1.736	1.736
Z	2	2
Mu (mm-1)	1.432	1.432
F000	796.0	796.0
F000’	792.98	
h,k,lmax	12,13,17	12,13,17
Nref	6059	6045
Tmin,Tmax	0.741,0.854	0.741,0.854
Tmin’	0.712	

```
Correction method= # Reported T Limits: Tmin=0.741 Tmax=0.854
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.000

R(reflections)= 0.0330( 5060)     wR2(reflections)= 0.0991( 6045)

S = 1.052                 Npar= 421
```

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 C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.72 Report
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.3 Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 1 N Ueq(max)/Ueq(min) Range	3.6 Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	O2 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C9 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	N5 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C8 Check
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .	98 Ang3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.005 Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cd1 -- O3 ..	9.8 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of N13A is Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N13B is Constrained at	0.5 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)..	2 % Note
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	155 Do !
	CD2 -N14 -N15 -N16 18.00 0.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	156 Do !
	CD2 -N14 -N15 -N16 -25.00 16.00 2.675 1.555 1.555 1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	141 Check
	N13B -N12 -N13A 1.555 1.555 1.555 41.60 Deg.	
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

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Datablock 1 - ellipsoid plot