

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: b

Bond precision: C-C = 0.0034 Å Wavelength=0.71073

Cell: a=6.1802(11) b=11.754(2) c=12.715(2)
 alpha=90 beta=102.782(2) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	900.8(3)	900.8(3)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	C18 H16 Cu N2 O8	?
Sum formula	C18 H16 Cu N2 O8	C18 H16 Cu N2 O8
Mr	451.88	451.87
Dx,g cm-3	1.666	1.666
Z	2	2
Mu (mm-1)	1.265	1.265
F000	462.0	462.0
F000'	462.87	
h,k,lmax	7,14,15	7,14,15
Nref	1685	1635
Tmin,Tmax	0.746,0.817	0.688,0.823
Tmin'	0.661	

Correction method= MULTI-SCAN

Data completeness= 0.970 Theta(max)= 25.500

R(reflections)= 0.0302(1342) wR2(reflections)= 0.0767(1635)

S = 1.037 Npar= 135


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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full	Low	0.970
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C4	- C7 ...	1.53 Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C5	- C6 ...	1.53 Ang.

	Alert level G	
PLAT004_ALERT_5_G	Info: Polymeric Structure Found with Dimension .	2
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	?
PLAT007_ALERT_5_G	Note: Number of Unrefined D-H Atoms	1
PLAT128_ALERT_4_G	Alternate Setting of Space-group P21/c	P21/n
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	3
	N1 -CU1 -N1 -C1 16.00 0.00 3.556 1.555 1.555 1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	6
	N1 -CU1 -N1 -C5 3.00 0.00 3.556 1.555 1.555 1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	7
	O1 -CU1 -O1 -C6 172.10 0.20 3.556 1.555 1.555 1.555	
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Cu1 (II)	2.28

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
4 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. 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*, 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.

