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: 5

Bond precision: C-C = 0.0040 A Wavelength=0.71070

Cell: a=22.3521(7) b=13.8512(4) c=13.9977(4)
alpha=90 beta=118.433(3) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	3811.0(2)	3811.0(2)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	?
Moiety formula	C22 H30 Co2 N23 O5, N3, 4(H2 O)	C22 H30 Co2 N23 O5, N3, 4(H2 O)
Sum formula	C22 H38 Co2 N26 O9	C22 H38 Co2 N26 O9
Mr	928.64	928.64
Dx,g cm-3	1.618	1.619
Z	4	4
Mu (mm-1)	0.955	0.955
F000	1912.0	1912.0
F000’	1915.37	
h,k,lmax	27,17,17	27,17,17
Nref	3887	3882
Tmin,Tmax	0.795,0.909	0.978,1.000
Tmin’	0.751	

Correction method= # Reported T Limits: Tmin=0.978 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.320

R(reflections)= 0.0402(3113) wR2(reflections)= 0.1064(3882)

S = 1.064 Npar= 289

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 B

PLAT420_ALERT_2_B	D-H Without Acceptor	O2W	--H4	.	Please Check

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Alert level C

PLAT414_ALERT_2_C	Short Intra D-H..H-X	H6A	..H10B		1.98 Ang.
			x,y,z =		1_555 Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N6	--H6A	.	Please Check

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Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				6 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...				1 Report
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF				Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms				6 Report
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group	C2/c			I2/a Note
PLAT300_ALERT_4_G	Atom Site Occupancy of O3	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N10	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N11	Constrained at			0.5 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)				8% Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #				87 Check
	N11 -N11 -N10	5.656	1.555	5.656	29.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #				89 Check
	N11 -N10 -N11	1.555	1.555	5.656	13.70 Deg.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #				2 Note
	N3				
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #				3 Note
	H2 O				
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #				4 Note
	H2 O				
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				12 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL				2018 Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
11 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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_PLAT420_5
;
PROBLEM: D-H Without Acceptor       O2W      --H4       .     Please Check
RESPONSE: H atoms positions have been determined from difference Fourier synthesis and refined.
;
# end Validation Reply Form
```

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.

PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock 5 - ellipsoid plot