

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CAN_2

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: CAN_2

Bond precision: C-C = 0.0056 Å Wavelength=0.71073

Cell: a=10.068(4) b=15.632(5) c=15.399(5)
 alpha=90 beta=98.588(7) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2396.4(14)	2396.4(14)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H16 Co N2 O4, C3 H6 O	?
Sum formula	C27 H22 Co N2 O5	C27 H22 Co N2 O5
Mr	513.40	513.39
Dx,g cm-3	1.423	1.423
Z	4	4
Mu (mm-1)	0.757	0.757
F000	1060.0	1060.0
F000'	1061.83	
h,k,lmax	12,18,18	11,18,18
Nref	4262	4250
Tmin,Tmax	0.947,0.978	0.934,0.978
Tmin'	0.934	

Correction method= # Reported T Limits: Tmin=0.934 Tmax=0.978
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.088

R(reflections)= 0.0493(2860) wR2(reflections)= 0.1248(4250)

S = 1.024 Npar= 318

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

PLAT018_ALERT_1_C	_diffn_measured_fraction_theta_max .NE. *_full	! Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1C Check
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H12A ..01C .	2.73 Ang.
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .	37 Ang**3
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.597	12 Report
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0 Info



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C2C Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.12 Ratio
PLAT794_ALERT_5_G	Tentative Bond Valency for Co1 (II) .	1.87 Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	47% Note

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

- 3 **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
2 **ALERT type 3** Indicator that the structure quality may be low
4 **ALERT type 4** Improvement, methodology, query or suggestion
2 **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* 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.

Datablock CAN_2 - ellipsoid plot

