

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CAN_1dCHCl3

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_1dCHCl3

Bond precision: C-C = 0.0040 Å

Wavelength=0.71073

Cell: a=10.0048(16) b=16.371(3) c=15.036(3)
 alpha=90 beta=97.402(3) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	2442.2(8)	2442.3(7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H16 Co N2 O4, C H0.84 Cl3	?
Sum formula	C25 H16.84 Cl3 Co N2 O4	C25 H16.83 Cl3 Co N2 O4
Mr	574.52	574.52
Dx, g cm-3	1.563	1.562
Z	4	4
Mu (mm-1)	1.066	1.066
F000	1163.4	1163.0
F000'	1166.93	
h,k,lmax	13,21,20	13,21,20
Nref	6087	6062
Tmin,Tmax	0.764,0.889	0.707,0.888
Tmin'	0.703	

Correction method= # Reported T Limits: Tmin=0.707 Tmax=0.888

AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 28.310

R(reflections)= 0.0479(4504)

wR2(reflections)= 0.1293(6062)

S = 1.019

Npar= 326

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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		C1C Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C11C	0.131 Check
PLAT977_ALERT_2_C	Check Negative Difference Density on H1C		-0.34 eA-3



Alert level G

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: C25 H16.83 Cl3 Col N2 O4
Atom count from the _atom_site data: C25 H16.84 Cl3 Col N2 O4

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3 Info
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical		? Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Col	--O2B_b	6.1 s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		25% Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .		1.12 Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		110 Check
	CL4C -C1C -CL3C	1.555 1.555 1.555	13.40 Deg.
PLAT794_ALERT_5_G	Tentative Bond Valency for Col	(II)	1.82 Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	25 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		13 Info

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

4 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
0 ALERT type 3 Indicator that the structure quality may be low
5 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

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.

