

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ip1_167

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: ip1_167

Bond precision: C-C = 0.0070 A Wavelength=0.71073

Cell: a=7.8532(16) b=10.000(2) c=13.192(3)
 alpha=90 beta=105.06(3) gamma=90

Temperature: 210 K

	Calculated	Reported
Volume	1000.4(4)	1000.4(3)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	C2 H11 Co N3 O5, N O3, H2 O	?
Sum formula	C2 H13 Co N4 O9	C2 H13 Co N4 O9
Mr	296.09	296.09
Dx, g cm ⁻³	1.966	1.966
Z	4	4
Mu (mm ⁻¹)	1.764	1.764
F000	608.0	608.0
F000'	609.76	
h,k,lmax	10,13,17	10,13,17
Nref	2433	2403
Tmin,Tmax	0.535,0.884	0.424,0.593
Tmin'	0.489	

Correction method= MULTI-SCAN

Data completeness= 0.988 Theta(max)= 28.080

R(reflections)= 0.0525(1520) wR2(reflections)= 0.1327(2403)

S = 0.881 Npar= 197

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

PLAT242_ALERT_2_B Low

Ueq as Compared to Neighbors for

N4 Check

Alert level C

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 3.1 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0070 Ang.
PLAT417_ALERT_2_C Short Inter D-H..H-D H2B .. H8A .. 2.11 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1C .. O8 .. 2.66 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H2A .. O6 .. 2.63 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H3A .. O1 .. 2.65 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.928 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 6 Report
PLAT976_ALERT_2_C Check Calcd Residual Density 0.57A From O6 -0.44 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density 0.82A From O7 -0.43 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density 0.99A From O5 -0.42 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 18 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 3 Report
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 3 Do !
N2 -CO1 -O1 -C1 5.00 3.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 9 Do !
N3 -CO1 -O2 -C2 -7.00 2.00 1.555 1.555 1.555 1.555
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3 Note
H2 O
PLAT860_ALERT_3_G Number of Least-Squares Restraints 33 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 24 Note

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

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

PLATON version of 20/08/2014; check.def file version of 18/08/2014

