

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_CHEM0913

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: mo_CHEM0913

Bond precision: C-C = 0.0049 A

Wavelength=0.71073

Cell: a=10.7131(7) b=16.1974(11) c=16.5188(11)
 alpha=118.419(2) beta=93.901(2) gamma=100.021(2)
Temperature: 158 K

	Calculated	Reported
Volume	2444.6(3)	2444.6(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C112 H100, 4(C2 H4 Cl2)	C112 H100, 4(C2 H4 Cl2)
Sum formula	C120 H116 Cl8	C120 H116 Cl8
Mr	1841.65	1841.72
Dx,g cm-3	1.251	1.251
Z	1	1
Mu (mm-1)	0.281	0.281
F000	972.0	972.0
F000'	973.45	
h,k,lmax	13,20,20	13,20,20
Nref	9656	9602
Tmin,Tmax	0.964,0.981	0.416,0.745
Tmin'	0.958	

Correction method= # Reported T Limits: Tmin=0.416 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.994

Theta(max)= 26.056

R(reflections)= 0.0789(5553)

wR2(reflections)= 0.2356(9602)

S = 1.034

Npar= 630

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**

PLAT230_ALERT_2_C	Hirshfeld Test Diff for C23 --C25 .	5.2 s.u.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C23	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Cl3_4	0.105 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Cl3_5	0.105 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00492 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.933 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	13 Report

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	20 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8 Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002 Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	8 Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	2 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)	100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	5.45 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)	5.61 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 4)	2.12 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 5)	0.42 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 6)	2.39 Check
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C1 -C7_a .	1.44 Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C11 -C16 .	1.42 Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	40 Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	57 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	38 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3 Info

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

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

