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: ll5182-c2m

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

Cell: a=22.8164(11) b=13.3547(3) c=16.4024(8)
alpha=90 beta=133.376(9) gamma=90
Temperature: 153 K

	Calculated	Reported
Volume	3632.8(6)	3632.8(6)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	C40 H94 Co6 N8 O18, 2(Cl O4), 2(C2 H6 O), 2(H2 O)	C40 H94 Co6 N8 O18, 2(Cl O4), 2(C2 H6 O), 2(H2 O)
Sum formula	C44 H110 Cl2 Co6 N8 O30	C44 H110 Cl2 Co6 N8 O30
Mr	1655.88	1655.88
Dx,g cm-3	1.514	1.514
Z	2	2
Mu (mm-1)	1.493	1.493
F000	1732.0	1732.0
F000’	1737.52	
h,k,lmax	27,15,19	27,15,19
Nref	3363	3357
Tmin,Tmax	0.685,0.764	0.697,0.775
Tmin’	0.672	

Correction method= # Reported T Limits: Tmin=0.697 Tmax=0.775
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.010

R(reflections)= 0.0311(3139) wR2(reflections)= 0.0807(3357)

S = 1.071 Npar= 244

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

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PLAT245_ALERT_2_C U(iso) H111    Smaller than U(eq) O11     by ...      0.029 AngSq
PLAT420_ALERT_2_C D-H Without Acceptor       N2     --  H2B    ...     Please Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3 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 ..............          8 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      10.35 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group     C2/m       I2/m Note
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        Cl1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H6A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H6B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H6C    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H12A   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H12B   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H12C   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C13    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H13A   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H13B   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H142   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H143   is Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =          11 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.50) in Resd. #          4 Check
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C5     -   C6     ..       1.51 Ang.
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         35 Do !
            O1  -CO1 -O1  -C1     74.26  0.16   2.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         41 Do !
            O1  -CO1 -O1  -CO2  -141.46  0.06   2.555   1.555   1.555   5.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         92 Do !
            O6  -CO3 -O4  -C5    180.00  0.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        103 Do !
            N2  -CO3 -O5  -C7   -142.60  0.80   6.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        109 Do !
            N2  -CO3 -O5  -CO2   -12.50  0.90   6.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        131 Do !
            O5  -CO3 -N2  -C8     14.80  0.90   6.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        138 Do !
            O4  -CO3 -O6  -C11     0.00  0.00   1.555   1.555   1.555   1.555
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.12 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          8 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 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
  2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 31 ALERT level G = General information/check it is not something unexpected

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  6 ALERT type 2 Indicator that the structure model may be wrong or deficient
  1 ALERT type 3 Indicator that the structure quality may be low
 24 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.

PLATON version of 06/05/2016; check.def file version of 05/05/2016

Datablock ll5182-c2m - ellipsoid plot