checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MG6_sq

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: MG6_sq

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Bond precision:  C-C = 0.0037 A          Wavelength=0.71073

Cell:          a=13.0056(9)      b=13.5507(9)     c=15.7196(11)
               alpha=74.740(2)   beta=67.413(2)   gamma=62.618(2)
Temperature:   150 K
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	Calculated	Reported
Volume	2258.6(3)	2258.6(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C48 H34 Cl4 Co N6 [+ solvent]	?
Sum formula	C48 H34 Cl4 Co N6 [+ solvent]	C48 H34 Cl4 Co N6 O0
Mr	895.54	895.54
Dx,g cm-3	1.317	1.317
Z	2	2
Mu (mm-1)	0.656	0.656
F000	918.0	918.0
F000’	920.12	
h,k,lmax	16,16,19	16,17,20
Nref	8857	8715
Tmin,Tmax	0.737,0.849	0.691,0.849
Tmin’	0.704	

```
Correction method= # Reported T Limits: Tmin=0.691 Tmax=0.849
AbsCorr = MULTI-SCAN

Data completeness= 0.984          Theta(max)= 25.999

R(reflections)= 0.0432( 7478)     wR2(reflections)= 0.1243( 8715)

S = 1.091                  Npar= 534
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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

```
PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ...          ! Note
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Alert level C

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PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        9.0 Ratio
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N5       --Hn5      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N6       --Hn6      .     Please Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          8 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        129 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          4 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
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Alert level G

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CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C48 H34 Cl4 Co N6 O0
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         96.00     96.00    0.00
           H         68.00     68.00    0.00
           Cl         8.00      8.00    0.00
           Co         2.00      2.00    0.00
           N         12.00     12.00    0.00
           O          2.00      0.00    2.00
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          2 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.002 Degree
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          2 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Co        (II)      .       2.24 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! 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          6 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         20 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.5 Low
PLAT954_ALERT_1_G Reported (CIF) and Actual (FCF) Kmax Differ by .          1 Units
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .          1 Units
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          8 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  17 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
   4 ALERT type 4 Improvement, methodology, query or suggestion
   3 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.

PLATON version of 03/06/2021; check.def file version of 02/06/2021

Datablock MG6_sq - ellipsoid plot