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: exp_123

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

Cell:          a=8.1448(2)        b=8.2664(3)       c=8.4973(3)
               alpha=102.314(3)   beta=101.136(2)   gamma=95.278(2)
Temperature:   293 K
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	Calculated	Reported
Volume	543.10(3)	543.10(3)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C6 H24 Co N6, C4 H4 O6, Cl, 5(H2 O)	C6 H24 Co N6, C4 H4 O6, 5(H2 O), Cl
Sum formula	C10 H38 Cl Co N6 O11	C10 H38 Cl Co N6 O11
Mr	512.84	512.84
Dx,g cm-3	1.568	1.568
Z	1	1
Mu (mm-1)	0.976	0.976
F000	272.0	272.0
F000’	272.63	
h,k,lmax	10,10,10	11,11,12
Nref	4454[2227]	4391
Tmin,Tmax		0.908,1.000
Tmin’		

```
Correction method= # Reported T Limits: Tmin=0.908 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.97/0.99      Theta(max)= 26.370

R(reflections)= 0.0178( 4381)     wR2(reflections)= 0.0464( 4391)

S = 1.049                 Npar= 280
```

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 A

EXPT005_ALERT_1_A _exptl_crystal_description is missing
Crystal habit description.
The following tests will not be performed.
CRYSR_01
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value ..... Please Do !

Alert level B

PLAT035_ALERT_1_B _chemical_absolute_configuration Info Not Given Please Do !

Alert level C

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 7.95 Note

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Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 24 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Co1 --N1 . 5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Co1 --N3 . 5.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Co1 --N6 . 6.6 s.u.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 4 Note
H2 O
PLAT791_ALERT_4_G Model has Chirality at C8 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C9 (Sohnke SpGr) S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Co1 (III) . 3.37 Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 7 Note
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ -2 Units

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

10 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
1 ALERT type 3 Indicator that the structure quality may be low
3 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 05/12/2020; check.def file version of 05/12/2020

Datablock exp_123 - ellipsoid plot