checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

```
Bond precision:   C-C = 0.0052 A          Wavelength=0.71073

Cell:          a=10.923(2)        b=12.278(3)       c=14.169(4)
               alpha=84.505(13)   beta=86.603(11)   gamma=78.723(11)
Temperature:   295 K
```

	Calculated	Reported
Volume	1853.4(8)	1853.5(8)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C33 H26 Co N5 O5, 2(F6 P), H2 O	C33 H28 Co1 F12 N5 O6 P2
Sum formula	C33 H28 Co F12 N5 O6 P2	C33 H28 Co1 F12 N5 O6 P2
Mr	939.47	939.47
Dx,g cm-3	1.683	1.683
Z	2	2
Mu (mm-1)	0.662	0.662
F000	948.0	948.0
F000'	949.77	
h,k,lmax	13,15,17	13,15,17
Nref	7139	7076
Tmin,Tmax	0.876,0.905	0.890,0.910
Tmin'	0.876	

```
Correction method= # Reported T Limits: Tmin=0.890 Tmax=0.910
AbsCorr = NUMERICAL

Data completeness= 0.991            Theta(max)= 25.816

R(reflections)= 0.0509( 5406)                    wR2(reflections)=
                                                 0.0933( 5406)
S = 1.000                  Npar= 532
```

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

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O4 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        P1       0.131 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O6       0.149 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         32 Report
```

Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of         P1 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of         P2 Check
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O4       .      106.6 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O5       .      106.4 Degree
PLAT769_ALERT_4_G CIF Embedded explicitly supplied scattering data     Please Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
            F6 P
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (III)     .       3.51 Info
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         50 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked          ! Info
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...        492 Check
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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
   6 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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   4 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 12/09/2022; check.def file version of 09/08/2022

Datablock I - ellipsoid plot

