checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20241127-zs_auto

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: 20241127-zs_auto

Bond precision: C-C = 0.0047 A Wavelength=1.54184

Cell: a=11.6744(2) b=21.7762(4) c=9.08477(18)
alpha=90 beta=106.474(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2214.76(7)	2214.75(8)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C20 H19.50 Co K N2 O7), 2(C H4 O)	C40 H39 Co2 K2 N4 O14, 2(C H4 O)
Sum formula	C42 H47 Co2 K2 N4 O16	C42 H47 Co2 K2 N4 O16
Mr	1059.90	1059.89
Dx,g cm-3	1.589	1.589
Z	2	2
Mu (mm-1)	8.214	8.214
F000	1094.0	1094.0
F000'	1089.44	
h,k,lmax	14,27,11	14,26,11
Nref	4765	4622
Tmin,Tmax	0.906,0.921	0.391,1.000
Tmin'	0.849	

Correction method= # Reported T Limits: Tmin=0.391 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.970 Theta(max)= 78.449

R(reflections)= 0.0754(4195) wR2(reflections)= 0.1681(4622)

S = 1.095 Npar= 302

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

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C20 H19.50 Co K N2 O7), 2(C H4 O)
             Rep.: C40 H39 Co2 K2 N4 O14, 2(C H4 O)
PLAT414_ALERT_2_C Short Intra D-H..H-X       H2       ..H1AD     .       1.98 Ang.
                                                    x,y,z  =      1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.500 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          6 Report
               3  0  0,   2 25  1,   9  0  6,   9  1  6,  -8  2 10,  -8  4 10,
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.91Ang From O2      .      -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2        .      -0.41 eA-3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          6 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          2 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
             H2
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      15.14 Why ?
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.          3 Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
             C1A     C1B     C2A     C2B     H1AA    H1B     H1AB    H2A
             H2B
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         6% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2       ..C1A      .       3.01 Ang.
                                          x,1/2-y,1/2+z  =      4_566 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         11 Note
             C0AA    C00Q    H1AA    H1AB    C1AA    H1AC    H1AD    H1AE
             H00A    H00B    H00C
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         19 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
               1  0  0,   0  2  0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        122 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          5 Note
               0  2  0,   3  0  0,   2 25  1,  -8  4 10,   1  0  0,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      6.518 Note
             Predicted wR2: Based on SigI**2  2.58 or SHELX Weight 15.35
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

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
20 **ALERT level G** = General information/check it is not something unexpected

2 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
   5 ALERT type 3 Indicator that the structure quality may be low
   7 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT042_20241127-zs_auto
;
PROBLEM: Calc. and Reported MoietyFormula Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT414_20241127-zs_auto
;
PROBLEM: Short Intra D-H..H-X       H2       ..H1AD     .       1.98 Ang.
RESPONSE: ...
;
_vrf_PLAT906_20241127-zs_auto
;
PROBLEM: Large K Value in the Analysis of Variance ......      3.500 Check
RESPONSE: ...
;
_vrf_PLAT911_20241127-zs_auto
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600          6 Report
RESPONSE: ...
;
_vrf_PLAT976_20241127-zs_auto
;
PROBLEM: Check Calcd Resid. Dens.  0.91Ang From O2      .      -0.43 eA-3
RESPONSE: ...
;
_vrf_PLAT977_20241127-zs_auto
;
PROBLEM: Check Negative Difference Density on H2        .      -0.41 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

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 02/02/2025; check.def file version of 02/02/2025

Datablock 20241127-zs_auto - ellipsoid plot