checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound1

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: Compound1

Bond precision:  C-C = 0.0028 Å  Wavelength=0.7107 Å

Cell:  
\[ a=12.6929(10) \]
\[ b=22.7763(19) \]
\[ c=23.8472(19) \]
\[ \alpha=90^\circ \]
\[ \beta=90^\circ \]
\[ \gamma=90^\circ \]

Temperature:  100 K

| Calculated  | Reported  |
|-------------|-----------|
| Volume 6894.2(10) | 6894.2(10) |
| Space group F d d d | F d d d |
| Hall group -F 2uv 2vw | -F 2uv 2vw |
| Moiety formula C12 H10 Co N4 O4 [+ solvent] | C12 H10 Co N4 O4, (C3 H7 N O) |
| Sum formula C12 H10 Co N4 O4 [+ solvent] | C15 H17 Co N5 O5 |
| Mr 333.17 | 406.26 |
| Dx,g cm\(^{-3}\) 1.284 | 1.635 |
| Z 16 | 16 |
| Mu (mm\(^{-1}\)) 1.012 | 1.041 |
| F000 2704.0 | 3504.0 |
| F000' 2710.62 | |
| h,k,lmax 16,30,31 | 16,30,31 |
| Nref 2182 | 2112 |
| Tmin,Tmax 0.920,0.949 | 0.914,0.991 |
| Tmin' 0.920 | |

Correction method= # Reported T Limits: Tmin=0.914 Tmax=0.991 AbsCorr = NUMERICAL

Data completeness= 0.968 Theta(max)= 28.430

R(reflections)= 0.0344( 1706)  wR2(reflections)= 0.0900( 2112)

S = 1.038  Npar= 96
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**

**DENS01_ALERT_1_C** The ratio of the submitted crystal density and that
calculated from the formula is outside the range 0.99 <> 1.01
Crystal density given = 1.635
Calculated crystal density = 1.566

**PLAT046_ALERT_1_C** Reported Z, MW and D(calc) are Inconsistent ..... 1.566 Check

**PLAT250_ALERT_2_C** Large U3/U1 Ratio for Average U(i,j) Tensor ..... 2.1 Note

**Alert level G**

**FORM01_ALERT_2_G** There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: C15 H17 Co1 N5 O5
Atom count from the _atom_site data: C12 H10 Co1 N4 O4

**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  16
From the CIF: _chemical_formula_sum C15 H17 Co N5 O5
TEST: Compare cell contents of formula and atom_site data

| atom | Z*formula | cif sites | diff |
|------|-----------|-----------|------|
| C    | 240.00    | 192.00    | 48.00|
| H    | 272.00    | 160.00    | 112.00|
| Co   | 16.00     | 16.00     | 0.00 |
| N    | 80.00     | 64.00     | 16.00|
| O    | 80.00     | 64.00     | 16.00|

**PLAT004_ALERT_5_G** Polymeric Structure Found with Maximum Dimension

**PLAT007_ALERT_5_G** Number of Unrefined Donor-H Atoms .............. 2 Report

**PLAT014_ALERT_1_G** N.O.K. _shelx_fab_checksum Found in CIF ...... Please Check

**PLAT041_ALERT_1_G** Calc. and Reported SumFormula Strings Differ Please Check

**PLAT068_ALERT_1_G** Reported F000 Differences from Calcd (or Missing)...

**PLAT083_ALERT_2_G** SHELXL Second Parameter in WGHT Unusually Large 8.15 Why ?

**PLAT605_ALERT_4_G** Largest Solvent Accessible VOID in the Structure

**PLAT720_ALERT_4_G** Number of Unusual/Non-Standard Labels ............ 2 Note

**PLAT764_ALERT_4_G** Overcomplete CIF Bond List Detected (Rep/Expd) .

**PLAT794_ALERT_5_G** Tentative Bond Valency for Co1 (II) .

**PLAT869_ALERT_4_G** ALERTS Related to the Use of SQUEEZE Suppressed

**PLAT912_ALERT_4_G** Missing # of FCF Reflections Above STh/L= 0.600

**PLAT978_ALERT_2_G** Number C-C Bonds with Positive Residual Density.

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

7 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
0 ALERT type 3 Indicator that the structure quality may be low
5 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.

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PLATON version of 22/12/2019; check.def file version of 13/12/2019
