checkCIF/PLATON report

Structure factors have been supplied for datablock(s) User-defined

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: User-defined

Bond precision: C-C = 0.0088 A Wavelength=0.71075

Cell: a=7.0728(9) b=10.3625(13) c=12.0604(16)
alpha=67.284(4) beta=81.212(4) gamma=77.056(4)
Temperature: 106 K

	Calculated	Reported
Volume	792.48(18)	792.48(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H4 Co N10 O4, C4 H12 Co N2 O4, 6(H2 O)	C20 H28 Co2 N12 O14
Sum formula	C20 H28 Co2 N12 O14	C20 H28 Co2 N12 O14
Mr	778.40	778.38
Dx,g cm-3	1.631	1.631
Z	1	1
Mu (mm-1)	1.130	1.131
F000	398.0	398.0
F000’	398.88	
h,k,lmax	9,13,15	9,13,15
Nref	3640	3640
Tmin,Tmax	0.873,0.978	0.873,0.978
Tmin’	0.636	

Correction method= # Reported T Limits: Tmin=0.873 Tmax=0.978
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 27.491

R(reflections)= 0.0977(2163) wR2(reflections)= 0.2105(3698)

S = 1.109 Npar= 235

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

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PLAT417_ALERT_2_A Short Inter D-H..H-D       H6       ..H14      .       1.69 Ang.
                                                      x,y,z  =      1_555 Check
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Alert level B

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PLAT245_ALERT_2_B U(iso) H12       Smaller than U(eq) O6        by      0.062 Ang**2
PLAT417_ALERT_2_B Short Inter D-H..H-D       H11      ..H14      .       2.09 Ang.
                                                      x,y,z  =      1_555 Check
PLAT420_ALERT_2_B D-H Without Acceptor       O7       --H13      .     Please Check
PLAT482_ALERT_4_B Small D-H..A Angle Rep for O8       ..O5       .      86.60 Degree
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Alert level C

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PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00883 Ang.
PLAT417_ALERT_2_C Short Inter D-H..H-D       H2       ..H11      .       2.10 Ang.
                                                  1-x,-y,1-z  =      2_656 Check
PLAT417_ALERT_2_C Short Inter D-H..H-D       H2       ..H12      .       2.10 Ang.
                                                  1-x,-y,1-z  =      2_656 Check
PLAT417_ALERT_2_C Short Inter D-H..H-D       H4       ..H5       .       2.13 Ang.
                                                      x,y,z  =      1_555 Check
PLAT482_ALERT_4_C Small D-H..A Angle Rep for O7       ..O6       .      98.80 Degree
PLAT482_ALERT_4_C Small D-H..A Angle Rep for O7       ..O5       .      90.00 Degree
PLAT482_ALERT_4_C Small D-H..A Angle Rep for O8       ..O5       .      98.00 Degree
PLAT755_ALERT_4_C D-H     Calc     0.94000, Rep    0.943(4) ......  Senseless s.u.
             O3       -H1             1.555   1.555 ........     #   46 Check
PLAT755_ALERT_4_C D-H     Calc     0.94000, Rep    0.936(5) ......  Senseless s.u.
             O3       -H2             1.555   1.555 ........     #   46 Check
PLAT755_ALERT_4_C D-H     Calc     0.95000, Rep    0.953(5) ......  Senseless s.u.
             O4       -H3             1.555   1.555 ........     #   46 Check
PLAT755_ALERT_4_C D-H     Calc     0.94000, Rep    0.943(5) ......  Senseless s.u.
             O4       -H4             1.555   1.555 ........     #   46 Check
PLAT755_ALERT_4_C D-H     Calc     0.97000, Rep    0.966(5) ......  Senseless s.u.
             O5       -H5             1.555   1.555 ........     #   46 Check
PLAT755_ALERT_4_C D-H     Calc     0.98000, Rep    0.985(8) ......  Senseless s.u.
             O5       -H6             1.555   1.555 ........     #   46 Check
PLAT755_ALERT_4_C D-H     Calc     0.98000, Rep    0.985(8) ......  Senseless s.u.
             O5       -H6             1.555   1.555 ........     #   46 Check
PLAT755_ALERT_4_C D-H     Calc     0.97000, Rep   0.970(11) ......  Senseless s.u.
             O6       -H11            1.555   1.555 ........     #   46 Check
PLAT756_ALERT_4_C H...A   Calc     1.74000, Rep    1.735(3) ......  Senseless s.u.
             H1       -O1             1.555   1.555 ........     #   46 Check
PLAT756_ALERT_4_C H...A   Calc     1.73000, Rep    1.728(8) ......  Senseless s.u.
             H2       -O6             1.555   2.656 ........     #   46 Check
PLAT756_ALERT_4_C H...A   Calc     1.88000, Rep    1.880(5) ......  Senseless s.u.
             H3       -N1             1.555   1.555 ........     #   46 Check
PLAT756_ALERT_4_C H...A   Calc     1.75000, Rep    1.751(8) ......  Senseless s.u.
             H4       -O5             1.555   1.555 ........     #   46 Check
PLAT756_ALERT_4_C H...A   Calc     1.99000, Rep    1.993(4) ......  Senseless s.u.
             H5       -N2             1.555   2.665 ........     #   46 Check
PLAT758_ALERT_4_C D-H..A  Calc      172.00, Rep    172.2(3) ......  Senseless s.u.
             O3       -H1      -O1         1.555  1.555  1.555     #   76 Check
PLAT758_ALERT_4_C D-H..A  Calc      159.00, Rep    158.5(3) ......  Senseless s.u.
             O4       -H3      -N1         1.555  1.555  1.555     #   76 Check
PLAT758_ALERT_4_C D-H..A  Calc      162.00, Rep    161.6(3) ......  Senseless s.u.
             O4       -H4      -O5         1.555  1.555  1.555     #   76 Check
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PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     15.512 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.939 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.09A   From O5             0.61 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.05A   From O5            -0.51 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.04A   From O4            -0.46 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2              -0.31 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Info
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Alert level G

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CHEMS02_ALERT_1_G  Please check that you have entered the correct
           _publ_requested_category classification of your compound;
           FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
           FO or CO or EO for organic.
           From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or
           From the CIF: _chemical_formula_sum:C20 H28 Co2 N12 O14
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          9 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          9 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.004 Degree
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds          9 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          4 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O7         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O8         Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15        Constrained at       0.25 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        100% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .       1.97 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co2       (II)      .       2.02 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          6 Note
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).          4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          5 Note
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  30 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  21 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 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
  29 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
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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 20/08/2018; check.def file version of 20/08/2018

Datablock User-defined - ellipsoid plot