checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 12

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: 12

```
Bond precision:  C-C = 0.0266 A          Wavelength=0.71073

Cell:            a=14.4824(10)     b=14.4824(10)     c=28.280(4)
                 alpha=90          beta=90           gamma=120
Temperature:     150 K
```

	Calculated	Reported
Volume	5136.8(10)	5136.8(10)
Space group	P -3 1 c	P -3 1 c
Hall group	-P 3 2c	-P 3 2c
Moiety formula	2(C36 H21 Co Ir N3 O6), 0.333(C45 H33 Co3 N9 O6), 9(O)	?
Sum formula	C87 H53 Co3 Ir2 N9 O23	C87 H75 Co3 Ir2 N9 O23
Mr	2153.58	2175.75
Dx,g cm-3	1.392	1.407
Z	2	2
Mu (mm-1)	3.122	3.123
F000	2114.0	2158.0
F000’	2111.28	
h,k,lmax	18,18,35	18,18,35
Nref	3557	3528
Tmin,Tmax	0.408,0.855	0.364,0.752
Tmin’	0.377	

```
Correction method= # Reported T Limits: Tmin=0.364 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.992          Theta(max)= 26.454

R(reflections)= 0.0925( 3232)     wR2(reflections)= 0.2227( 3528)

S = 1.196                 Npar= 245
```

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.35A From O2W 3.88 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 2.39A From C13 -4.04 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.92A From O4W -3.73 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

Alert level B

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 22.17 Check

Author Response: All hydrogen atoms of the water molecules are not added due to the poor data set and heavily disorder. The reported formular includes these hydrogen atoms.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1W Check

Author Response: All hydrogen atoms of the water molecules are not added due to the poor data set and heavily disorder.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O4W Check

Author Response: All hydrogen atoms of the water molecules are not added due to the poor data set and heavily disorder.

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02658 Ang.

Author Response: This problem arises from the poor data set and heavily disorder.

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O1       ..O1W      .       2.61 Ang.
                                                    x,y,z  =      1_555 Check
```

Author Response: All hydrogen atoms of the water molecules are not added due to the poor data set and heavily disorder.

```
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  1.49A   From Co1             2.88 eA-3
```

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

Alert level C

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT213_ALERT_2_C Atom N1             has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom C6             has ADP max/min Ratio .....        3.5 prolat
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C4       --C12      .        6.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Co1      --O2       .       0.20 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         Ir1 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O4W      0.202 Check
PLAT430_ALERT_2_C Short Inter D...A Contact  O1W      ..O1W      .       2.90 Ang.
                                          1-x+y,2-x,z  =      3_675 Check
```

Author Response: All hydrogen atoms of the water molecules are not added due to the poor data set and heavily disorder.

```
PLAT430_ALERT_2_C Short Inter D...A Contact  O1W      ..O1W      .       2.90 Ang.
                                          2-y,1+x-y,z  =      2_765 Check
```

Author Response: All hydrogen atoms of the water molecules are not added due to the poor data set and heavily disorder.

```
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      8.887 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.296 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         23 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.13A   From O2              2.38 eA-3
```

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.81A   From O2              2.07 eA-3
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Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.12A From C17 2.03 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.85A From C5 1.99 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.63A From N2 1.92 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.29A From O4W 1.88 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.56A From C13 1.84 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.11A From O2W 1.78 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.85A   From C12   1.72 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.73A   From C14   1.69 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.49A   From C15   1.53 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.34A   From C20   1.53 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.50A   From Co1   -2.22 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.49A   From Co1   -2.08 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.23A   From O2W   -1.56 eA-3

Author Response: The [Co(terpy)(H2O)2] cations locating in the lattice are disordered over three symmetry-equivalent positions. We have carefully found out and fixed the whole molecule, but there are still a few unassigned large residue peaks due to the poor data set and heavily disorder.

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PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.01A   From O4W           -0.78 eA-3
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Alert level G

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FORMU01_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:C87 H75 Co3 Ir2 N9 O23
           Atom count from the _atom_site data:  C87.00347 H53.00390 Co3.004900 I
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    2
          From the CIF: _chemical_formula_sum  C87 H75 Co3 Ir2 N9 O23
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        174.00    174.00    0.00
          H        150.00    106.00   44.00
          Co         6.00      6.00    0.00
          Ir         4.00      4.00    0.00
          N         18.00     18.00    0.00
          O         46.00     48.00   -2.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         19 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         27 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     161.68 Why ?
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          1 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          9 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          6 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          3 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Co2        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2W        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3W        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2         Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3         Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20        Constrained at     0.3333 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  2  )         100% Note
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C1       -C6              0.17 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #          89 Check
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              CO2  -N2   -O2W     1.555   1.555   2.665              4.00 Deg.
PLAT780_ALERT_1_G Coordinates do not Form a Properly Connected Set     Please Do !
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .       1.02 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       246 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     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         2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        24 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         4 Info
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   3 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  30 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  45 ALERT level G = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  39 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
  29 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 10/08/2020; check.def file version of 06/08/2020

Datablock 12 - ellipsoid plot