checkCIF/PLATON report

Structure factors have been supplied for datablock(s) compound1, compound2

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 = 0.0081 A Wavelength=0.71073

Cell: a=10.5320(6) b=13.2619(7) c=18.1118(10)
alpha=70.883(5) beta=74.056(5) gamma=85.860(4)
Temperature: 298 K

	Calculated	Reported
Volume	2297.9(2)	2297.9(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C76 H52 Co5 O44 [+ solvent]	C76 H52 O36 Co5 12H2O 2Nh2(Ch3)2+
Sum formula	C76 H52 Co5 O44 [+ solvent]	C80 H92 Co5 N2 O48
Mr	1963.83	2144.20
Dx,g cm-3	1.419	1.550
Z	1	1
Mu (mm-1)	0.974	0.985
F000	995.0	1105.0
F000’	997.33	
h,k,lmax	14,18,24	14,18,24
Nref	12543	10439
Tmin,Tmax	0.652,0.752	0.974,1.000
Tmin’	0.636	

Correction method= # Reported T Limits: Tmin=0.974 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.832 Theta(max)= 29.270

R(reflections)= 0.0847(5537) wR2(reflections)= 0.1883(10439)

S = 1.211 Npar= 565

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 B

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PLAT430_ALERT_2_B Short Inter D...A Contact  O2       ..O2       .       2.77 Ang.
                                              -x,1-y,1-z  =      2_566 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O2W      ..O5       .       2.69 Ang.
                                             -1-x,2-y,-1-z  =      2_474 Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).         14 Note
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Alert level C

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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
PLAT213_ALERT_2_C Atom O10             has ADP max/min Ratio .....        3.7 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O11 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O12 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O15 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Co2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Co3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C27 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00806 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H2B      ..H8       .       1.98 Ang.
                                               x,y,z  =      1_555 Check
PLAT430_ALERT_2_C Short Inter D...A Contact  O4W      ..O14      .       2.85 Ang.
                                              -2-x,1-y,1-z  =      2_366 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         32 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.89A   From O4W             0.44 eA-3
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C80 H92 Co5 N2 O48
           Atom count from _chemical_formula_moiety:C1540 H1180 Co10240 N20 O760
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:C80 H92 Co5 N2 O48
           Atom count from the _atom_site data:  C76 H52 Co5 O44
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    1
          From the CIF: _chemical_formula_sum  C80 H92 Co5 N2 O48
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         80.00     76.00    4.00
          H         92.00     52.00   40.00
          Co         5.00      5.00    0.00
          N          2.00      0.00    2.00
          O         48.00     44.00    4.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
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PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .       1.98 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co2       (II)      .       1.83 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co3       (II)      .       1.95 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       2059 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.6 Low
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.          0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  15 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  18 ALERT level G = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
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Datablock: compound2

Bond precision: C-C = 0.0076 A Wavelength=0.71073

Cell: a=11.2564(6) b=15.9785(9) c=16.5583(10)
       alpha=62.347(6) beta=73.527(5) gamma=70.219(5)
Temperature: 298 K

	Calculated	Reported
Volume	2453.6(3)	2453.6(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C41 H26 Co3 N O23 [+ solvent]	C82 H52 Co6 O36 10 H2O 2[(CH3)2CHNO]
Sum formula	C41 H26 Co3 N O23 [+ solvent]	C82 H86 Co6 N2 O48
Mr	1077.42	2221.10
Dx,g cm-3	1.458	1.503
Z	2	1
Mu (mm-1)	1.083	1.086
F000	1088.0	1138.0
F000’	1090.71	
h,k,lmax	15,21,22	14,20,20
Nref	13311	11189
Tmin,Tmax	0.640,0.754	0.992,1.000
Tmin’	0.627	

Correction method= # Reported T Limits: Tmin=0.992 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.841 Theta(max)= 29.211

R(reflections)= 0.0663(6840) wR2(reflections)= 0.1559(11189)

S = 1.175 Npar= 613

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 B

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 10.0 Ratio
PLAT220_ALERT_2_B NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 7.0 Ratio
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C39 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of O19 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N1 Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 17 Note
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check

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Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.86 Report
PLAT213_ALERT_2_C Atom O15 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C39 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C41 has ADP max/min Ratio ..... 3.2 oblate
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Co2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Co3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C36 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.1 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00759 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 26 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.81A From O1W 0.43 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.10A From O3W 0.42 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.86A From O1W 0.42 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.01A From O3W 0.42 eA-3

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C82 H86 Co6 N2 O48
Atom count from _chemical_formula_moiety:C164 H108 Co12 O7224
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:C82 H86 Co6 N2 O48
Atom count from the _atom_site data: C82 H52 Co6 N2 O46
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

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          From the CIF: _cell_formula_units_Z    1
          From the CIF: _chemical_formula_sum  C82 H86 Co6 N2 O48
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         82.00     82.00    0.00
          H         86.00     52.00   34.00
          Co         6.00      6.00    0.00
          N          2.00      2.00    0.00
          O         48.00     46.00    2.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         1 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         1 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         3 Info
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      2.00 Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C39 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C40 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for        C41 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C40      - C41_h    .      1.76 Ang.
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.14 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C40      --C41           1.76 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C41      --C40           1.76 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .     1.96 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co2       (II)      .     2.12 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co3       (II)      .     2.01 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         7 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      1746 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       1.6 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ          2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ          2 Units
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.         1 Info
```

```
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   5 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

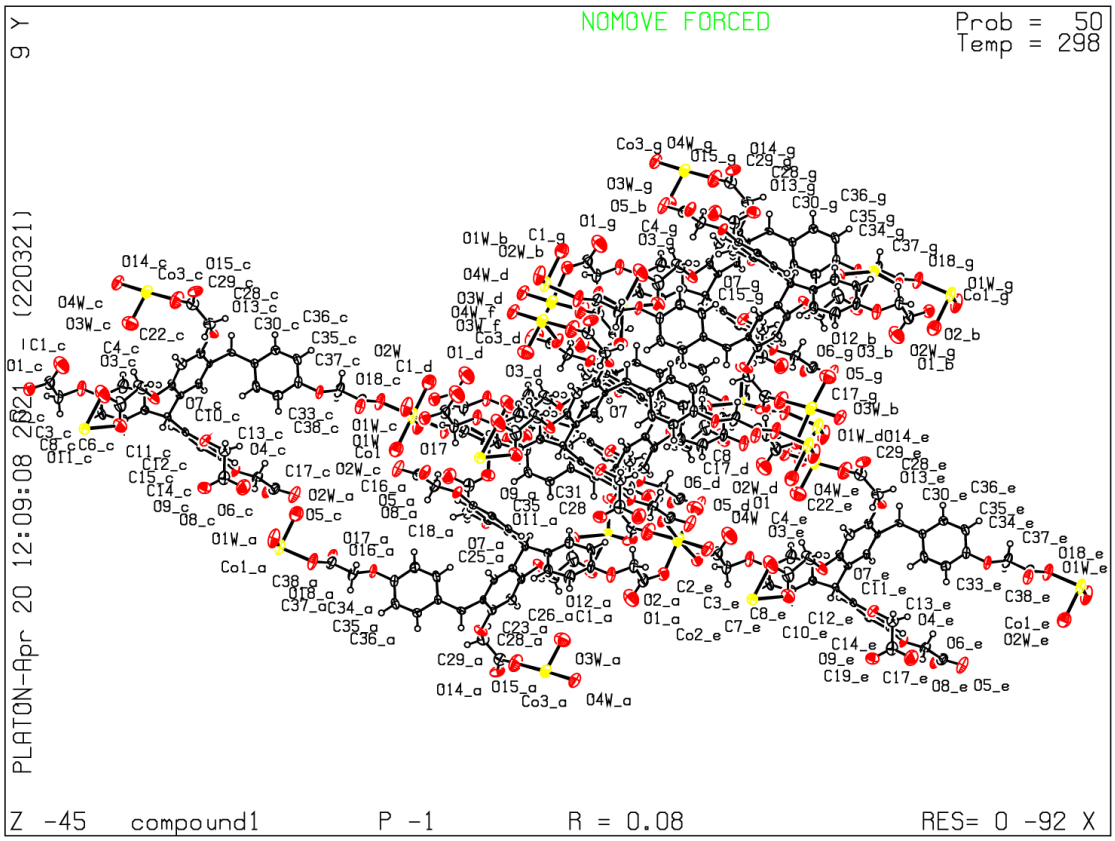
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 22/03/2021; check.def file version of 19/03/2021

Datablock compound1 - ellipsoid plot



Datablock compound2 - ellipsoid plot

