checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dmwmsv6-73_sq

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: dmwmsv6-73_sq

Bond precision: C-C = 0.0045 A   Wavelength=0.68890

Cell: a=32.85880(17)   b=30.06718(13)   c=40.1053(2)
                 alpha=90   beta=96.0585(5)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	39401.6(3)	39401.6(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C336 H262 Co8 N72), C6 Cl4 O2, 2(B2 F5), 14.34(B F4) [+ solve	C336 H262 Co8 N72, 3.584(B2 F8), B2 F5, 0.25(C12 Cl8 O4)
Sum formula	C678 H524 B18.34 Cl4 Co16 F67.36 N144 O2 [+ solvent]	C377 H416 B16 Cl2 Co8 F64 N72 O39
Mr	13283.23	8511.09
Dx,g cm-3	1.120	1.435
Z	2	4
Mu (mm-1)	0.378	0.415
F000	13627.9	17600.0
F000'	13644.80	
h,k,lmax	47,43,58	47,43,58
Nref	62835	62714
Tmin,Tmax		0.975,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.975 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.998   Theta(max)= 29.947

R(reflections)= 0.0827(36940)   wR2(reflections)= 0.3038(62714)

S = 1.091   Npar= 2167

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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PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor ....        4.5 Note
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          4 Check
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Alert level C
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PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.30 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.39 Report
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl23      0.186 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F92      0.126 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F22      0.131 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F32      0.129 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F42      0.156 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
            C336 H262 Co8 N72
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         76 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          7 Check
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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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:   C377 H416 B16 Cl2 Co8 F64 N72
            Atom count from _chemical_formula_moiety:C339 H262 B9.167999 Cl2 Co8 F
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:C377 H416 B16 Cl2 Co8 F64 N72 O3
            Atom count from the _atom_site data:  C339 H262 B9.17 Cl2 Co8 F33.6799
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
              not performed for this radiation type.
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    4
            From the CIF: _chemical_formula_sum  C377 H416 B16 Cl2 Co8 F64 N72 O39
            TEST: Compare cell contents of formula and atom_site data

            atom    Z*formula  cif sites diff
            C       1508.00   1356.00  152.00
            H       1664.00   1048.00  616.00
            B         64.00     36.68   27.32
            Cl         8.00      8.00    0.00
            Co        32.00     32.00    0.00
            F        256.00    134.72  121.28
            N        288.00    288.00    0.00
            O        156.00      4.00  152.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       223 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       240 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
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ  Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.50 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.18 Report
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PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka      0.68890 Ang.
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..............      0.00013 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............      0.00020 Ang.
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records            3 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records            4 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records            4 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records           30 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records            1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records            1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records            1 Report
PLAT244_ALERT_4_G Low     'Solvent' Ueq as Compared to Neighbors of        B11 Check
PLAT244_ALERT_4_G Low     'Solvent' Ueq as Compared to Neighbors of        B21 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl23          Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl24          Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl25          Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl26          Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O21G          Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O22G          Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11G          Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12G          Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13G          Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14G          Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15G          Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16G          Constrained at       0.25 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )      100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  6         4.24 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  7         3.68 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for       C24D Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl24     ..C53F            3.06 Ang.
                                              x,y,z  =     1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl24     ..C54F            3.18 Ang.
                                              x,y,z  =     1_555 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure       ! Info
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        741 Check
           B91  -F93  -B91     1.555   1.555    2.856          38.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        742 Check
           B91  -F94  -B91     2.856   1.555    1.555          34.80 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         12 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
           C6 Cl4 O2
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
           B2 F5
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
           B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
           B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
           B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7 Note
           B F4
PLAT794_ALERT_5_G Tentative Bond Valency for Co1        (II)     .     1.53 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co2        (II)     .     1.54 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co3        (II)     .     1.52 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co4        (II)     .     1.50 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          8 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............     5560 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 !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600          44 Note
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PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....        2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...       36 Note
PLAT984_ALERT_1_G The Co-f'=     0.3538 Deviates from the B&C-Value    0.3480 Check
PLAT985_ALERT_1_G The Co-f"=     0.9121 Deviates from the B&C-Value    0.9239 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  68 ALERT level G = General information/check it is not something unexpected

  11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  16 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
  43 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
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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_PLAT250_dmwmsv6-73_sq
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....        4.5 Note
RESPONSE: ...
;
_vrf_PLAT934_dmwmsv6-73_sq
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          4 Check
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.

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