checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 1

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Bond precision:  C-C = 0.0133 A          Wavelength=0.71073

Cell:            a=21.312(10)     b=21.312(10)     c=16.548(3)
                 alpha=90         beta=90          gamma=90
Temperature:     113 K

                Calculated                Reported
Volume          7516(7)                   7516(5)
Space group     I -4 2 d                  I -4 2 d
Hall group      I -4 2bw                  ?
Moiety formula  C48 H32 Cl5 Mn6 N24, 4(O) C48 H41 Cl5 Mn6 N24 O4
Sum formula     C48 H32 Cl5 Mn6 N24 O4    C48 H41 Cl5 Mn6 N24 O4
Mr              1515.87                   1524.89
Dx,g cm-3       1.340                     1.340
Z               4                         4
Mu (mm-1)       1.207                     1.207
F000            3020.0                    3052.0
F000'           3031.65
h,k,lmax        27,27,21                  27,27,21
Nref            4465[ 2428]               4451
Tmin,Tmax       0.805,0.865               0.805,0.865
Tmin'           0.786

Correction method= MULTI-SCAN

Data completeness= 1.83/1.00      Theta(max)= 27.810

R(reflections)= 0.0843( 3863)     wR2(reflections)= 0.2198( 4451)

S = 1.080                 Npar= 192
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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

PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 2139 Ang3

Alert level B

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

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
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.174
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.470
From the CIF: _refine_ls_abs_structure_Flack_su 0.050
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 ..... 0.174
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ? Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ? Check
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0133 Ang.

Alert level G

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:C48 H41 Cl5 Mn6 N24 O4
Atom count from the _atom_site data: C48 H32 Cl5 Mn6 N24 O4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C48 H41 Cl5 Mn6 N24 O4
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	192.00	192.00	0.00
H	164.00	128.00	36.00
Cl	20.00	20.00	0.00
Mn	24.00	24.00	0.00
N	96.00	96.00	0.00
O	16.00	16.00	0.00

PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension . 3
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ? Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ ? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.11
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as . mixed
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 2 Units
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 5
CL3 -MN1 -CL1 -MN1 107.70 0.70 1.555 1.555 1.555 4.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 10
CL3 -MN1 -CL1 -MN1 -155.10 0.60 1.555 1.555 1.555 3.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 15
CL3 -MN1 -CL1 -MN1 -57.80 0.60 1.555 1.555 1.555 2.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 20
CL1 -MN1 -CL3 -MN2 -26.90 0.70 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 25
CL3 -MN2 -CL3 -MN1 96.49 0.05 5.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 52
N2 -MN2 -N5 -N4 17.00 4.00 5.555 1.555 1.555 1.555

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PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         57
            N2  -MN2 -N5  -C1   -154.00  3.00   5.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         84
            N5  -MN2 -N2  -N1    156.00  3.00   5.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         89
            N5  -MN2 -N2  -C12   -27.00  4.00   5.555   1.555   1.555   1.555
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.28 Ratio
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  1 ALERT level A = Most likely a serious problem - resolve or explain
  1 ALERT level B = A potentially serious problem, consider carefully
  8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 19 ALERT level G = General information/check it is not something unexpected

  8 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
  4 ALERT type 3 Indicator that the structure quality may be low
 11 ALERT type 4 Improvement, methodology, query or suggestion
  2 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*, 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 01/06/2013; check.def file version of 24/05/2013

Datablock 1 - ellipsoid plot