checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ata649c

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: ata649c

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Bond precision:  C-C = 0.0253 A          Wavelength=0.71073

Cell:            a=21.8159(3)     b=21.8159(3)     c=18.6491(7)
                 alpha=90         beta=90          gamma=90
Temperature:     120 K
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	Calculated	Reported
Volume	8875.7(4)	8875.7(6)
Space group	P 4 c c	P 4 c c
Hall group	P 4 -2c	P 4 -2c
Moiety formula	C48 H52 Mn4 N4 O20 Y, 2(C16 H36 N), Cl O4	C48 H52 Mn3.64 N4 O20 Y, 0.36(Mn1), 0.5(Cl2 O8), 2(C16 H36 N)
Sum formula	C80 H124 Cl Mn4 N6 O24 Y	C80 H124 Cl Mn4 N6 O24 Y
Mr	1897.97	1897.96
Dx,g cm-3	1.420	1.420
Z	4	4
Mu (mm-1)	1.305	1.305
F000	3976.0	3976.0
F000’	3972.42	
h,k,lmax	26,26,23	26,24,23
Nref	8739[4522]	8346
Tmin,Tmax	0.770,0.889	0.759,0.857
Tmin’	0.760	

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Correction method= # Reported T Limits: Tmin=0.759 Tmax=0.857
AbsCorr = INTEGRATION

Data completeness= 1.85/0.96      Theta(max)= 25.996

R(reflections)= 0.0762( 6181)     wR2(reflections)= 0.1983( 8346)

S = 1.072                  Npar= 571
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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

PLAT234_ALERT_4_A Large Hirshfeld Difference C39 --C40 0.39 Ang.

Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual) Mn1A Check

Author Response: The metallacrowns are disordered over two position, with a free refined ratio of 0.91 to 0.09. Due to the low side occupation factor of the second position, only the manganese atoms were refined over two postions.

PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual) Mn2A Check

Author Response: The metallacrowns are disordered over two position, with a free refined ratio of 0.91 to 0.09. Due to the low side occupation factor of the second position, only the manganese atoms were refined over two postions.

PLAT413_ALERT_2_A Short Inter XH3 .. XHn H28A ..H32B 1.83 Ang.

Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

Alert level B

PLAT234_ALERT_4_B Large Hirshfeld Difference C38 --C39 0.26 Ang.

Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C27 Check
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02529 Ang.

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 integration
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 7.90 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.01 Report
PLAT220_ALERT_2_C Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 3.8 Ratio

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PLAT221_ALERT_2_C Solv./Anion  Resd 3  C   Ueq(max)/Ueq(min) Range        4.5 Ratio
PLAT223_ALERT_4_C Solv./Anion  Resd 3  H   Ueq(max)/Ueq(min) Range        5.7 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for   C27      --C28       .        5.3 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mn1A     --O2               0.16 Ang.
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Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

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PLAT234_ALERT_4_C Large Hirshfeld Difference Mn2      --O7_g             0.17 Ang.
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Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

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PLAT234_ALERT_4_C Large Hirshfeld Difference Mn2A     --O10              0.18 Ang.
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Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

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PLAT234_ALERT_4_C Large Hirshfeld Difference Mn2A     --O7_g             0.22 Ang.
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Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

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PLAT234_ALERT_4_C Large Hirshfeld Difference Mn2A     --O8_g             0.16 Ang.
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Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

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PLAT234_ALERT_4_C Large Hirshfeld Difference Mn2A     --C19_g            0.19 Ang.
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Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

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PLAT234_ALERT_4_C Large Hirshfeld Difference C31      --C32              0.22 Ang.
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Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

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PLAT234_ALERT_4_C Large Hirshfeld Difference C37      --C38              0.20 Ang.
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Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

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PLAT234_ALERT_4_C Large Hirshfeld Difference Cl1      --O12             0.23 Ang.
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Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

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PLAT234_ALERT_4_C Large Hirshfeld Difference Cl1      --O13             0.24 Ang.
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Author Response: The n-Bu~4~N cation is disordered over several positions, which cannot be modelled satisfactorily. Therefore, only the main component was refined without any disorder.

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C26 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C39 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        Cl1 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C27      - C28      .       1.38 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C31      - C32      .       1.41 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C35      - C36      .       1.43 Ang.
PLAT361_ALERT_2_C Long  C(sp3)-C(sp3) Bond  C21      - C23      ..       1.68 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          5 Report
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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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         22 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         16 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      32.87 Why ?
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...         -2 Units
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          5 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          3 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O11        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O12        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O13        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O14        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         5% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  2  )         5% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )        80% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  O11      ..C38              2.96 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O12      ..C40              2.95 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C28      ..C32              3.07 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        199 Check
              O13  -CL1  -O12     1.555   1.555   2.655            43.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        201 Check
              O13  -CL1  -O12     2.655   1.555   1.555            43.20 Deg.
PLAT794_ALERT_5_G Tentative Bond Valency for Y1        (III)     .       3.37 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Y2        (III)     .       3.43 Info
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PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        159 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           2 Units
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .          1 Units
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   4 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  30 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  26 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  24 ALERT type 2 Indicator that the structure model may be wrong or deficient
   8 ALERT type 3 Indicator that the structure quality may be low
  24 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 23/04/2018; check.def file version of 23/04/2018

Datablock ata649c - ellipsoid plot