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: abs

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Bond precision:  C-C = 0.0061 A          Wavelength=1.54184

Cell:          a=36.3787(4)   b=16.16213(17)       c=14.51853(16)
               alpha=90       beta=101.5137(10)    gamma=90
Temperature:   123 K
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	Calculated	Reported
Volume	8364.50(16)	8364.49(16)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C16 Al F36 O4, C40 H60 Ag Mo4 P12, 2(C0.22 H0.43 Cl0.43), 4(C0.	Al C16 F36 O4, C40 H60 Ag Mo4 P12, 3.45(C0.29 H0.58 Cl0.58)
Sum formula	C57 H62 Ag Al Cl2 F36 Mo4 O4 P12	C57 H62 Ag Al Cl2 F36 Mo4 O4 P12
Mr	2456.22	2456.21
Dx,g cm-3	1.951	1.950
Z	4	4
Mu (mm-1)	10.624	10.624
F000	4808.0	4808.0
F000’	4841.02	
h,k,lmax	45,20,18	45,19,17
Nref	8442	8226
Tmin,Tmax	0.439,0.516	0.435,0.617
Tmin’	0.271	

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Correction method= GAUSSIAN

Data completeness= 0.974          Theta(max)= 73.708

R(reflections)= 0.0413( 7474)     wR2(reflections)= 0.1167( 8226)

S = 1.067                 Npar= 738
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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 B

Crystal system given = monoclinic

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 4 Report

Author Response: 4 atoms of a disordered tert-butyl group with 51% occupancy were kept isotropic during the refinement. Otherwise the displacement parameters of these atoms adopted very unrealistic values.

PLAT213_ALERT_2_B Atom F29 has ADP max/min Ratio ..... 4.4 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_B Atom F34 has ADP max/min Ratio ..... 4.5 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_B Atom F36 has ADP max/min Ratio ..... 4.2 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_B Atom C56 has ADP max/min Ratio ..... 4.6 oblate

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) Range 6.9 Ratio

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

Alert level C

PLAT213_ALERT_2_C Atom F19 has ADP max/min Ratio ..... 3.9 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F21 has ADP max/min Ratio ..... 3.7 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F27 has ADP max/min Ratio ..... 3.2 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F4 has ADP max/min Ratio ..... 3.2 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F7 has ADP max/min Ratio ..... 3.3 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F9 has ADP max/min Ratio ..... 3.2 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F32 has ADP max/min Ratio ..... 3.1 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom C52 has ADP max/min Ratio ..... 3.5 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT220_ALERT_2_C Large Non-Solvent F Ueq(max)/Ueq(min) Range 3.6 Ratio

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT234_ALERT_4_C Large Hirshfeld Difference C49 -- C50 .. 0.25 Ang.

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion. The ternary C atom of the tert-butyl groups are not as heavily concerned by the motion.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... Al4 Check

Author Response: Al is the central atom of a heavily disordered anion with large displacement parameters.

Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          6 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          4 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      36.36 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          4 Report
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         36 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F25    --  C52     ..         6.2 su
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F27    --  C52     ..         5.6 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo1    --  P2      ..         5.4 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo1    --  P3      ..         5.4 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo1    --  P4      ..         6.0 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo1    --  P5      ..         5.2 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo1    --  P6      ..         6.8 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo2    --  P1      ..         6.0 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo2    --  P2      ..         5.2 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo2    --  P3      ..         5.4 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo2    --  P4      ..         5.4 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo2    --  P5      ..         6.4 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo2    --  P6      ..         6.4 su
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =          49 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =         100 Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C9 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....  C16 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....  C20 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....    ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............  109 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  29 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  32 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
  10 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 20/08/2014; check.def file version of 18/08/2014

Datablock abs - ellipsoid plot