checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: sw195

Bond precision: C-C = 0.0163 A   Wavelength=1.54178

Cell: a=29.608(5)   b=14.382(5)   c=35.671(5)
               alpha=90   beta=111.924(5)   gamma=90
Temperature: 110 K

	Calculated	Reported
Volume	14091(6)	14091(6)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C56 H40 Cu2 Mo8 O16 P8, 2(C16 Al F36 O4), 4(C H2 Cl2)	C56 H40 Cu2 Mo8 O16 P8, 2(C16 Al F36 O4), 4(C H2 Cl2)
Sum formula	C92 H48 Al2 Cl8 Cu2 F72 Mo8 O24 P8	C92 H48 Al2 Cl8 Cu2 F72 Mo8 O24 P8
Mr	4385.25	4385.25
Dx,g cm-3	2.067	2.067
Z	4	4
Mu (mm-1)	9.782	9.782
F000	8464.0	8464.0
F000'	8501.09	
h,k,lmax	33,16,40	33,16,40
Nref	11142	10747
Tmin,Tmax	0.225,0.738	0.222,0.738
Tmin'	0.080	

Correction method= MULTI-SCAN

Data completeness= 0.965   Theta(max)= 62.170

R(reflections)= 0.0667(7936)   wR2(reflections)= 0.1856(10747)

S = 0.999   Npar= 973

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
PLAT242_ALERT_2_A Check Low   Ueq as Compared to Neighbors for   Al1

Author Response: Depending on their position the atoms in the fluorinated alkoxyaluminate are affected differently by the thermal motion of the anion.

🟠 Alert level B

```
THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =    0.5736
PLAT213_ALERT_2_B Atom F33     has ADP max/min Ratio .............      4.20 prola
PLAT241_ALERT_2_B Check High     Ueq as Compared to Neighbors for        O10
PLAT241_ALERT_2_B Check High     Ueq as Compared to Neighbors for        O11
PLAT241_ALERT_2_B Check High     Ueq as Compared to Neighbors for        O12
PLAT242_ALERT_2_B Check Low      Ueq as Compared to Neighbors for        C29
```

Author Response: Depending on their position the atoms in the fluorinated alkoxyaluminate are affected differently by the thermal motion of the anion.

```
PLAT242_ALERT_2_B Check Low      Ueq as Compared to Neighbors for        C31
```

Author Response: Depending on their position the atoms in the fluorinated alkoxyaluminate are affected differently by the thermal motion of the anion.

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PLAT242_ALERT_2_B Check Low      Ueq as Compared to Neighbors for        C42
```

Author Response: Depending on their position the atoms in the fluorinated alkoxyaluminate are affected differently by the thermal motion of the anion.

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PLAT234_ALERT_4_B Large Hirshfeld Difference F2     -- C33     ..      0.22  Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference F5     -- C34     ..      0.21  Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference F6     -- C34     ..      0.21  Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference F30    -- C42     ..      0.23  Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference F36    -- C44     ..      0.20  Ang.
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🟡 Alert level C

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PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......    0.96
PLAT213_ALERT_2_C Atom F7      has ADP max/min Ratio .............    3.30 prola
PLAT213_ALERT_2_C Atom F28     has ADP max/min Ratio .............    3.70 prola
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...    3.19 Ratio
PLAT220_ALERT_2_C Large Non-Solvent    F     Ueq(max)/Ueq(min) ...    3.14 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for     F8    -- C35    ..     5.91 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for     F32   -- C43    ..     5.08 su
PLAT241_ALERT_2_C Check High     Ueq as Compared to Neighbors for       O9
PLAT242_ALERT_2_C Check Low      Ueq as Compared to Neighbors for       C30
```

Author Response: Depending on their position the atoms in the fluorinated alkoxyaluminate are affected differently by the thermal motion of the anion.

```
PLAT242_ALERT_2_C Check Low      Ueq as Compared to Neighbors for       C32
```

Author Response: Depending on their position the atoms in the fluorinated alkoxyaluminate are affected differently by the thermal motion of the anion.

```
PLAT242_ALERT_2_C Check Low        Ueq as Compared to Neighbors for        C43
```

Author Response: Depending on their position the atoms in the fluorinated alkoxyaluminate are affected differently by the thermal motion of the anion.

```
PLAT242_ALERT_2_C Check Low        Ueq as Compared to Neighbors for        C44
```

Author Response: Depending on their position the atoms in the fluorinated alkoxyaluminate are affected differently by the thermal motion of the anion.

```
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ...        16
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C32    -   C43   ...       1.43 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C32    -   C44   ...       1.70 Ang.
PLAT432_ALERT_2_C Short Inter X...Y Contact  F19    ..  C15    ..       2.95 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .     94.00 A**3
PLAT153_ALERT_1_C The su's on the Cell Axes   are Equal (x 100000)      500 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo1    --  C3     ..       0.11  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo1    --  C4     ..       0.12  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo1    --  C11    ..       0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo1    --  C12    ..       0.13  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo2    --  C13    ..       0.11  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo3    --  C16    ..       0.12  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo3    --  C25    ..       0.13  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo3    --  C26    ..       0.13  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo4    --  C27    ..       0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo4    --  C28    ..       0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1     --  C11    ..       0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O2     --  C12    ..       0.13  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O5     --  C25    ..       0.14  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O6     --  C26    ..       0.12  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O7     --  C27    ..       0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O8     --  C28    ..       0.14  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C17    --  C18    ..       0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F1     --  C33    ..       0.20  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F27    --  C41    ..       0.17  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F29    --  C42    ..       0.19  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C29    --  C33    ..       0.19  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C29    --  C34    ..       0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31    --  C39    ..       0.17  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31    --  C40    ..       0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31    --  C41    ..       0.16  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C32    --  C42    ..       0.19  Ang.
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⬤ Alert level G
```
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        42
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         4
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  1 ALERT level A = In general: serious problem
 13 ALERT level B = Potentially serious problem
 44 ALERT level C = Check and explain
  2 ALERT level G = General alerts; check

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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23 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
32 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check
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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 12/11/2008; check.def file version of 12/11/2008

Datablock sw195 - ellipsoid plot