checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: sw213

Bond precision: C-C = 0.0178 A   Wavelength=1.54178

Cell: a=15.4622(3)   b=21.5487(2)   c=27.0717(9)
                 alpha=90   beta=90.820(2)   gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	9019.1(4)	9019.1(4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H20 Mo4 O8 P4, 2(C16 Al F36 O4)	C28 H20 Mo4 O8 P4, 2(C16 Al F36 O4)
Sum formula	C60 H20 Al2 F72 Mo4 O16 P4	C60 H20 Al2 F72 Mo4 O16 P4
Mr	2926.36	2926.36
Dx,g cm-3	2.155	2.155
Z	4	4
Mu (mm-1)	7.295	7.295
F000	5640.0	5640.0
F000'	5673.35	
h,k,lmax	17,24,31	17,24,31
Nref	14364	14305
Tmin,Tmax	0.347,0.536	0.355,0.733
Tmin'	0.125	

Correction method= ANALYTICAL

Data completeness= 0.996   Theta(max)= 62.440

R(reflections)= 0.0711(9040)   wR2(reflections)= 0.2067(14305)

S = 0.943   Npar= 1423

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   C46

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_A Check Low        Ueq as Compared to Neighbors for        C58
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_A Check Low        Ueq as Compared to Neighbors for        C59
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_A Check Low        Ueq as Compared to Neighbors for        C60
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

🔴 **Alert level B**
```
PLAT230_ALERT_2_B Hirshfeld Test Diff for     F10    -- C36    ..       8.78 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for     F17    -- C38    ..      11.41 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for     F27    -- C41    ..       8.75 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for     F46    -- C52    ..       9.30 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for     F51    -- C53    ..       9.23 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for     F54    -- C54    ..       8.04 su
PLAT241_ALERT_2_B Check High       Ueq as Compared to Neighbors for        O13
PLAT241_ALERT_2_B Check High       Ueq as Compared to Neighbors for        O15
PLAT241_ALERT_2_B Check High       Ueq as Compared to Neighbors for        C52
PLAT241_ALERT_2_B Check High       Ueq as Compared to Neighbors for        C54
PLAT242_ALERT_2_B Check Low        Ueq as Compared to Neighbors for        C30
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

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

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_B Check Low        Ueq as Compared to Neighbors for        C50
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT234_ALERT_4_B Large Hirshfeld Difference F18    -- C38    ..       0.29 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C30    -- C38    ..       0.29 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference F47    -- C52    ..       0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference F71    -- C60    ..       0.28 Ang.
```

🟡 **Alert level C**

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
            Calculated sin(theta_max)/wavelength =    0.5750
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....     3.50
PLAT213_ALERT_2_C Atom F12     has ADP max/min Ratio .............     3.10 prola
PLAT213_ALERT_2_C Atom C38     has ADP max/min Ratio .............     3.40 prola
PLAT213_ALERT_2_C Atom F40     has ADP max/min Ratio .............     3.60 prola
PLAT213_ALERT_2_C Atom F64     has ADP max/min Ratio .............     3.20 prola
PLAT213_ALERT_2_C Atom F65     has ADP max/min Ratio .............     3.90 prola
PLAT213_ALERT_2_C Atom F72     has ADP max/min Ratio .............     3.50 prola
PLAT213_ALERT_2_C Atom C52     has ADP max/min Ratio .............     3.20 prola
PLAT213_ALERT_2_C Atom C54     has ADP max/min Ratio .............     3.40 prola
PLAT220_ALERT_2_C Large Non-Solvent    C    Ueq(max)/Ueq(min) ...     3.16 Ratio
PLAT220_ALERT_2_C Large Non-Solvent    C    Ueq(max)/Ueq(min) ...     2.83 Ratio
PLAT220_ALERT_2_C Large Non-Solvent    F    Ueq(max)/Ueq(min) ...     3.40 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F20   --  C39    ..     6.22 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F40   --  C50    ..     6.33 su
PLAT241_ALERT_2_C Check High     Ueq as Compared to Neighbors for      C4
PLAT241_ALERT_2_C Check High     Ueq as Compared to Neighbors for      C53
PLAT242_ALERT_2_C Check Low      Ueq as Compared to Neighbors for      Mo1
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

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

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_C Check Low      Ueq as Compared to Neighbors for      C33
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_C Check Low      Ueq as Compared to Neighbors for      C35
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_C Check Low      Ueq as Compared to Neighbors for      C36
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_C Check Low      Ueq as Compared to Neighbors for      C40
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_C Check Low        Ueq as Compared to Neighbors for        C45
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_C Check Low        Ueq as Compared to Neighbors for        C47
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_C Check Low        Ueq as Compared to Neighbors for        C48
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_C Check Low        Ueq as Compared to Neighbors for        C49
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_C Check Low        Ueq as Compared to Neighbors for        C55
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT242_ALERT_2_C Check Low        Ueq as Compared to Neighbors for        C57
```

Author Response: This is resulting from an unequal influence of thermal movement on the ADPs of different atoms.

```
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ...         18
PLAT431_ALERT_2_C Short Inter HL..A Contact  F12    .. O1     ..    2.86 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact  F43    .. O1     ..    2.84 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact  F55    .. O4     ..    2.87 Ang.
PLAT142_ALERT_4_C su on b - Axis Small or Missing (x 100000) .....     20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo1    -- C12    ..    0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O2     -- C12    ..    0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F5     -- C34    ..    0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F8     -- C35    ..    0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F12    -- C36    ..    0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F14    -- C37    ..    0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F33    -- C43    ..    0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F34    -- C44    ..    0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F36    -- C44    ..    0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F37    -- C49    ..    0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F38    -- C49    ..    0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F42    -- C50    ..    0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F58    -- C56    ..    0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F64    -- C58    ..    0.24 Ang.
```

Alert level G

```
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        6
PLAT128_ALERT_4_G Non-standard setting of Space-group P21/c   ....     P21/n
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.        P1
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.        P4
```

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   4 ALERT level A = In general: serious problem
  17 ALERT level B = Potentially serious problem
  48 ALERT level C = Check and explain
   4 ALERT level G = General alerts; check

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  48 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
  22 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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 19/05/2009; check.def file version of 13/05/2009

NOMOVE FORCED

Prob =   50
Temp = 123

38 Y

PLATON-Jun 14 21:07:00 2009 - (190509)

Z -76   sw213   P 21/n   R = 0.07   RES=   0 -102 X