

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: sw256II

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Bond precision:    C-C = 0.0054 Å

Wavelength=1.54178

Cell:                    a=13.4258(1)            b=7.3930(1)            c=19.6321(2)  
                          alpha=90            beta=126.611(1)        gamma=90  
Temperature:            123 K

|                        | Calculated        | Reported          |
|------------------------|-------------------|-------------------|
| Volume                 | 1564.17(4)        | 1564.17(4)        |
| Space group            | P 2/c             | P 2/c             |
| Hall group             | -P 2yc            | -P 2yc            |
| Moiety formula         | C14 H10 Mo2 O4 P2 | C14 H10 Mo2 O4 P2 |
| Sum formula            | C14 H10 Mo2 O4 P2 | C14 H10 Mo2 O4 P2 |
| Mr                     | 496.04            | 496.04            |
| Dx, g cm <sup>-3</sup> | 2.106             | 2.106             |
| Z                      | 4                 | 4                 |
| Mu (mm <sup>-1</sup> ) | 15.201            | 15.201            |
| F000                   | 960.0             | 960.0             |
| F000'                  | 963.73            |                   |
| h,k,lmax               | 16,9,23           | 16,9,23           |
| Nref                   | 2972              | 2970              |
| Tmin,Tmax              | 0.021,0.050       | 0.039,0.222       |
| Tmin'                  | 0.003             |                   |

Correction method= GAUSSIAN

Data completeness= 0.999

Theta(max)= 70.070

R(reflections)= 0.0276( 2955)

wR2(reflections)= 0.0740( 2970)

S = 1.169

Npar= 200

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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.

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### Alert level B

|                   |                           |     |    |    |    |          |
|-------------------|---------------------------|-----|----|----|----|----------|
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for   | O2  | -- | C7 | .. | 7.89 su  |
| PLAT232_ALERT_2_B | Hirshfeld Test Diff (M-X) | Mo1 | -- | C7 | .. | 10.06 su |

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### Alert level C

|                   |                         |    |    |     |    |         |
|-------------------|-------------------------|----|----|-----|----|---------|
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for | O3 | -- | C13 | .. | 5.55 su |
|-------------------|-------------------------|----|----|-----|----|---------|

|                   |  |     |    |      |    |      |      |
|-------------------|--|-----|----|------|----|------|------|
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X)                  | Mo2 | -- | C13  | .. | 7.95 | su   |
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X)                  | Mo2 | -- | C14  | .. | 6.05 | su   |
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X)                  | Mo2 | -- | P2_b | .. | 5.07 | su   |
| PLAT141_ALERT_4_C | su on a - Axis Small or Missing (x 100000) |     |    |      |    | 10   | Ang. |



#### Alert level G

|                   |  |    |
|-------------------|--|----|
| 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. | P2 |

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- 0 **ALERT level A** = In general: serious problem
  - 2 **ALERT level B** = Potentially serious problem
  - 5 **ALERT level C** = Check and explain
  - 2 **ALERT level G** = General alerts; check
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- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  - 6 ALERT type 2 Indicator that the structure model may be wrong or deficient
  - 0 ALERT type 3 Indicator that the structure quality may be low
  - 3 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.

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PLATON version of 13/08/2009; check.def file version of 12/08/2009

