

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw204V

| | | | |
|-----------------|--|--|--------------|
| Bond precision: | C-C = 0.0190 A | Wavelength=1.54184 | |
| Cell: | a=35.7454(3) | b=19.1292(2) | c=38.5910(4) |
| | alpha=90 | beta=90 | gamma=90 |
| Temperature: | 100 K | | |
| | Calculated | Reported | |
| Volume | 26387.8(4) | 26387.8(4) | |
| Space group | P b c n | P b c n | |
| Hall group | -P 2n 2ab | -P 2n 2ab | |
| Moiety formula | C112 H80 In4 Mo16 O32 P16, 4(C16 Al F36 O4), 2(C H2 Cl2) | C112 H80 In4 Mo16 O32 P16, 4(C16 Al F36 O4), 2(C H2 Cl2) | |
| Sum formula | C178 H84 Al4 Cl4 F144 In4 Mo16 O48 P16 | C178 H84 Al4 Cl4 F144 In4 Mo16 O48 P16 | |
| Mr | 8466.01 | 8466.01 | |
| Dx,g cm-3 | 2.131 | 2.131 | |
| Z | 4 | 4 | |
| Mu (mm-1) | 11.701 | 11.708 | |
| F000 | 16240.0 | 16240.0 | |
| F000' | 16330.04 | | |
| h,k,lmax | 43,23,46 | 42,22,46 | |
| Nref | 24662 | 24448 | |
| Tmin,Tmax | 0.071,0.400 | 0.068,0.478 | |
| Tmin' | 0.001 | | |

Correction method= GAUSSIAN

Data completeness= 0.991 Theta(max)= 69.240

R(reflections)= 0.0849(17387) wR2(reflections)= 0.2648(24448)

S = 1.075 Npar= 1910

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

| | | |
|------------------------------|----------------------------------|------|
| PLAT241_ALERT_2_A Check High | Ueq as Compared to Neighbors for | 0201 |
| PLAT241_ALERT_2_A Check High | Ueq as Compared to Neighbors for | 0202 |
| PLAT241_ALERT_2_A Check High | Ueq as Compared to Neighbors for | 0203 |

| | | | |
|-------------------|---------------------------------|----------------------------------|-----------|
| PLAT242_ALERT_2_A | Check Low | Ueq as Compared to Neighbors for | Mo6A |
| PLAT242_ALERT_2_A | Check Low | Ueq as Compared to Neighbors for | C131 |
| PLAT242_ALERT_2_A | Check Low | Ueq as Compared to Neighbors for | C133 |
| PLAT242_ALERT_2_A | Check Low | Ueq as Compared to Neighbors for | A12 |
| PLAT242_ALERT_2_A | Check Low | Ueq as Compared to Neighbors for | C210 |
| PLAT242_ALERT_2_A | Check Low | Ueq as Compared to Neighbors for | C230 |
| PLAT242_ALERT_2_A | Check Low | Ueq as Compared to Neighbors for | C232 |
| PLAT234_ALERT_4_A | Large Hirshfeld Difference F2 | -- C111 .. | 0.33 Ang. |
| PLAT234_ALERT_4_A | Large Hirshfeld Difference F25 | -- C133 .. | 0.31 Ang. |
| PLAT234_ALERT_4_A | Large Hirshfeld Difference F62 | -- C233 .. | 0.35 Ang. |
| PLAT234_ALERT_4_A | Large Hirshfeld Difference C230 | -- C233 .. | 0.36 Ang. |



Alert level B

| | | | |
|-------------------|--------------------------------|----------------------------------|-----------|
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | F19 -- C131 .. | 8.71 su |
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | F65 -- C241 .. | 7.66 su |
| PLAT232_ALERT_2_B | Hirshfeld Test Diff (M-X) | Mo6A -- C37A .. | 11.56 su |
| PLAT241_ALERT_2_B | Check High | Ueq as Compared to Neighbors for | C5 |
| PLAT241_ALERT_2_B | Check High | Ueq as Compared to Neighbors for | O204 |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | Mo1 |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | Mo5B |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | Mo6B |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | A11 |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | C110 |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | C113 |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | C122 |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | C132 |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | C220 |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | C222 |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | C223 |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | C241 |
| PLAT242_ALERT_2_B | Check Low | Ueq as Compared to Neighbors for | C242 |
| PLAT234_ALERT_4_B | Large Hirshfeld Difference F3 | -- C111 .. | 0.25 Ang. |
| PLAT234_ALERT_4_B | Large Hirshfeld Difference F20 | -- C131 .. | 0.28 Ang. |
| PLAT234_ALERT_4_B | Large Hirshfeld Difference F24 | -- C132 .. | 0.29 Ang. |
| PLAT234_ALERT_4_B | Large Hirshfeld Difference F30 | -- C141 .. | 0.27 Ang. |
| PLAT234_ALERT_4_B | Large Hirshfeld Difference F39 | -- C211 .. | 0.28 Ang. |



Alert level C

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
 Weighted R factor given 0.265

| | | |
|-------------------|---|------------|
| PLAT084_ALERT_2_C | High R2 Value | 0.26 |
| PLAT213_ALERT_2_C | Atom P5B has ADP max/min Ratio | 3.20 prola |
| PLAT213_ALERT_2_C | Atom F4 has ADP max/min Ratio | 3.60 prola |
| PLAT213_ALERT_2_C | Atom F22 has ADP max/min Ratio | 3.10 oblat |
| PLAT213_ALERT_2_C | Atom F44 has ADP max/min Ratio | 3.10 prola |
| PLAT213_ALERT_2_C | Atom F61 has ADP max/min Ratio | 3.10 prola |
| PLAT213_ALERT_2_C | Atom F67 has ADP max/min Ratio | 3.20 prola |
| PLAT220_ALERT_2_C | Large Non-Solvent C Ueq(max)/Ueq(min) ... | 3.45 Ratio |
| PLAT220_ALERT_2_C | Large Non-Solvent O Ueq(max)/Ueq(min) ... | 3.92 Ratio |
| PLAT220_ALERT_2_C | Large Non-Solvent C Ueq(max)/Ueq(min) ... | 3.18 Ratio |
| PLAT222_ALERT_3_C | Large Non-Solvent H Ueq(max)/Ueq(min) ... | 3.46 Ratio |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for F27 -- C133 .. | 5.11 su |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for F56 -- C231 .. | 6.49 su |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for C210 -- C212 .. | 5.14 su |
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X) Mo5A -- C29A .. | 7.66 su |
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X) Mo5A -- C30A .. | 5.77 su |
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X) Mo6A -- P6A .. | 6.14 su |
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X) Mo6A -- C36A .. | 8.86 su |
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X) Mo6A -- C38A .. | 7.48 su |

| | | | |
|-------------------|--|----------------------------------|-----------|
| PLAT241_ALERT_2_C | Check High | Ueq as Compared to Neighbors for | P2 |
| PLAT241_ALERT_2_C | Check High | Ueq as Compared to Neighbors for | C2 |
| 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 | C7 |
| PLAT241_ALERT_2_C | Check High | Ueq as Compared to Neighbors for | C8 |
| PLAT241_ALERT_2_C | Check High | Ueq as Compared to Neighbors for | C15 |
| PLAT241_ALERT_2_C | Check High | Ueq as Compared to Neighbors for | O101 |
| PLAT241_ALERT_2_C | Check High | Ueq as Compared to Neighbors for | O102 |
| PLAT241_ALERT_2_C | Check High | Ueq as Compared to Neighbors for | O103 |
| PLAT241_ALERT_2_C | Check High | Ueq as Compared to Neighbors for | C111 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | In1 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | Mo2 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | Mo5A |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C40A |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C112 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C120 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C121 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C123 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C130 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C140 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C143 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C212 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C213 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C221 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C240 |
| PLAT242_ALERT_2_C | Check Low | Ueq as Compared to Neighbors for | C243 |
| PLAT313_ALERT_2_C | Oxygen with three covalent bonds (rare) | | O14A |
| PLAT313_ALERT_2_C | Oxygen with three covalent bonds (rare) | | O14B |
| PLAT313_ALERT_2_C | Oxygen with three covalent bonds (rare) | | O16A |
| PLAT313_ALERT_2_C | Oxygen with three covalent bonds (rare) | | O16B |
| PLAT342_ALERT_3_C | Low Bond Precision on C-C Bonds (x 1000) Ang .. | | 19 |
| PLAT431_ALERT_2_C | Short Inter HL..A Contact F23 .. O14B .. | | 2.84 Ang. |
| PLAT431_ALERT_2_C | Short Inter HL..A Contact F38 .. O14A .. | | 2.87 Ang. |
| PLAT432_ALERT_2_C | Short Inter X...Y Contact F59 .. C36B .. | | 2.87 Ang. |
| PLAT141_ALERT_4_C | su on a - Axis Small or Missing (x 100000) | | 30 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference Mo5A -- C31A .. | | 0.16 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference Mo5A -- C32A .. | | 0.16 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference Mo5A -- C33A .. | | 0.16 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference Mo5A -- C39A .. | | 0.18 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference Mo5A -- C40A .. | | 0.16 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference Mo6A -- C34A .. | | 0.18 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference O5 -- C25 .. | | 0.17 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference O9A -- C39A .. | | 0.21 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C1 -- C2 .. | | 0.23 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C1 -- C5 .. | | 0.23 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C2 -- C3 .. | | 0.18 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C15 -- C16 .. | | 0.16 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C17 -- C18 .. | | 0.15 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C20 -- C21 .. | | 0.16 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference F10 -- C121 .. | | 0.19 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference F32 -- C142 .. | | 0.19 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C110 -- C112 .. | | 0.19 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C120 -- C123 .. | | 0.15 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C130 -- C131 .. | | 0.17 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C140 -- C141 .. | | 0.18 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference F37 -- C211 .. | | 0.22 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference F40 -- C212 .. | | 0.22 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference F59 -- C232 .. | | 0.23 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference F66 -- C241 .. | | 0.18 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference F67 -- C242 .. | | 0.23 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C210 -- C211 .. | | 0.25 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C220 -- C222 .. | | 0.16 Ang. |

● **Alert level G**

| | |
|--|-------------|
| PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large.. | 0.19 |
| PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. | 9.06 |
| PLAT301_ALERT_3_G Note: Main Residue Disorder | 23.00 Perc. |
| PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints | 475 |
| PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus. | P2 |
| PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus. | P4 |
| PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus. | <P5B |
| PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of . | 144.00 A**3 |
| PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels | 2 |
| PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms | ! |

14 **ALERT level A** = In general: serious problem

23 **ALERT level B** = Potentially serious problem

83 **ALERT level C** = Check and explain

10 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

81 ALERT type 2 Indicator that the structure model may be wrong or deficient

5 ALERT type 3 Indicator that the structure quality may be low

43 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

Datablock sw204V - ellipsoid plot

