checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: sw80

Bond precision: C-C = 0.0121 A   Wavelength=1.54178

Cell: a=23.7788(1)   b=23.7788(1)   c=15.3445(1)
                  alpha=90   beta=90   gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	8676.26(8)	8676.26(8)
Space group	P -4	P -4
Hall group	P -4	P -4
Moiety formula	C73 H64 Ag2 N4 P4, 2(F6 P)	C73 H64 Ag2 N4 P4, 2(F6 P)
Sum formula	C73 H64 Ag2 F12 N4 P6	C73 H64 Ag2 F12 N4 P6
Mr	1626.85	1626.85
Dx,g cm-3	1.245	1.245
Z	4	4
Mu (mm-1)	5.207	5.207
F000	3288.0	3288.0
F000'	3305.40	
h,k,lmax	26,26,17	21,26,17
Nref	6521[12473]	10876
Tmin,Tmax	0.194,0.524	0.124,0.524
Tmin'	0.086	

Correction method= MULTI-SCAN

Data completeness= 1.67/0.87   Theta(max)= 58.930

R(reflections)= 0.0461(8680)   wR2(reflections)= 0.1215(10876)

S = 0.994   Npar= 862

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**
THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
          Calculated sin(theta_max)/wavelength =   0.5556
PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor 5.96

🟡 **Alert level C**

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PLAT230_ALERT_2_C Hirshfeld Test Diff for     C43    -- C48     ..     5.21 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for     C50    -- C51     ..     6.01 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for     C52    -- C53     ..     5.42 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for     C68    -- C69     ..     5.34 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)   Ag1    -- P1      ..     6.92 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)   Ag2    -- P1      ..     5.37 su
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds (x 1000) Ang ..      12
PLAT141_ALERT_4_C su on a - Axis Small or Missing (x 100000) .....      10 Ang.
PLAT143_ALERT_4_C su on c - Axis Small or Missing (x 100000) .....      10 Ang.
PLAT231_ALERT_4_C Hirshfeld Test (Solvent)    P5     -- F2      ..    7.38 su
PLAT231_ALERT_4_C Hirshfeld Test (Solvent)    P5     -- F4      ..    7.06 su
PLAT234_ALERT_4_C Large Hirshfeld Difference  N2     -- C18     ..    0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference  C5     -- C6      ..    0.15 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference  C12    -- C13     ..    0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference  C20    -- C21     ..    0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference  C53    -- C54     ..    0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference  C59    -- C60     ..    0.15 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference  C71    -- C72     ..    0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference  P6     -- F7      ..    0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference  P6     -- F8      ..    0.17 Ang.
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of      P5
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of      P6
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of      P8
PLAT950_ALERT_1_C Reported and Calculated Hmax Values Differ by ..      5
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⬤ Alert level G

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REFLT03_ALERT_1_G ALERT: Expected hkl max differ from CIF values
          From the CIF: _diffrn_reflns_theta_max        58.93
          From the CIF: _reflns_number_total            10876
          From the CIF: _diffrn_reflns_limit_ max hkl  19.  15.   17.
          From the CIF: _diffrn_reflns_limit_ min hkl  -21. -26.  -17.
          TEST1: Expected hkl limits for theta max
          Calculated maximum hkl   26.  26.   17.
          Calculated minimum hkl  -26. -26.  -17.
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
          correct. If it is not, please give the correct count in the
          _publ_section_exptl_refinement section of the submitted CIF.
          From the CIF: _diffrn_reflns_theta_max        58.93
          From the CIF: _reflns_number_total            10876
          Count of symmetry unique reflns        6521
          Completeness (_total/calc)         166.78%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured     4355
          Fraction of Friedel pairs measured    0.668
          Are heavy atom types Z>Si present       yes
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large.      0.14
PLAT033_ALERT_4_G Flack x Parameter Value Deviates from Zero .....      0.06
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure     !
PLAT792_ALERT_1_G The Model has Chirality at P2      (Verify) ....      S
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   0 ALERT level A = In general: serious problem
   2 ALERT level B = Potentially serious problem
  24 ALERT level C = Check and explain
   6 ALERT level G = General alerts; check

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
  19 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 29/06/2010; check.def file version of 26/06/2010

Datablock sw80 - ellipsoid plot