checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: sw253

Bond precision: C-C = 0.0111 A   Wavelength=1.54178

Cell: a=32.1751(3)   b=12.2014(2)   c=35.8672(5)
                  alpha=90   beta=99.675(1)   gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	13880.5(3)	13880.5(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H30 Cu Fe2 Mo2 O6 P10,	2 (C26 H30 CU FE2 MO2 O6
	C16 Al F36 O4	P10), 2 (C16 AL F36 O4)
Sum formula	C42 H30 Al Cu F36 Fe2 Mo2	C84 H60 AL2 CU2 F72 FE4
	O10 P10	MO4 O20 P20
Mr	2082.47	4164.94
Dx,g cm-3	1.993	1.993
Z	8	4
Mu (mm-1)	10.170	10.170
F000	8112.0	8112.0
F000'	8133.59	
h,k,lmax	38,14,42	38,14,42
Nref	24578	24417
Tmin,Tmax	0.336,0.835	0.413,0.839
Tmin'	0.254	

Correction method= ANALYTICAL

Data completeness= 0.993   Theta(max)= 66.680

R(reflections)= 0.0613(15220)   wR2(reflections)= 0.1730(24417)

S = 0.934   Npar= 1894

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**
PLAT230_ALERT_2_B Hirshfeld Test Diff for   O7   --   C37   ..   7.77 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cu1   --   P1   ..   12.52 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cu2   --   P11   ..   12.69 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cu2   --   P16   ..   14.56 su

Alert level C

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DIFMN02_ALERT_2_C  The minimum difference density is < -0.1*ZMAX*0.75
           _refine_diff_density_min given =      -3.477
           Test value =      -3.150
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT098_ALERT_2_C Large Reported Min.  (Negative) Residual Density     -3.48 eA-3
PLAT230_ALERT_2_C Hirshfeld Test Diff for     O6     --  C26     ..     6.88 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for     O11    --  C51     ..     6.36 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for     F20    --  C131    ..     5.07 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)   Mo1    --  C26     ..     7.46 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)   Cu1    --  P6      ..     7.76 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)   Cu1    --  C12     ..     7.34 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)   Cu1    --  C24     ..     5.80 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)   Mo3    --  P15     ..     5.30 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)   Mo3    --  C51     ..     9.03 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)   Mo4    --  C37     ..     6.89 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)   Cu2    --  C37     ..     6.68 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)   Cu2    --  C50     ..     8.39 su
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       Cu1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       Cu2
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       C230
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds (x 1000) Ang ..       11
PLAT431_ALERT_2_C Short Inter HL..A Contact   F2     ..  O2      ..     2.86 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact   F31    ..  O5      ..     2.76 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact   F49    ..  O8      ..     2.76 Ang.
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings  Differ       ?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ       ?
PLAT045_ALERT_1_C Calculated and Reported Z Differ by ............     2.00 Ratio
PLAT141_ALERT_4_C su on a - Axis Small or Missing (x 100000) .....       30 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo2    --  C11     ..     0.15 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cu1    --  C25     ..     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1     --  C11     ..     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O4     --  C24     ..     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O8     --  C38     ..     0.15 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F14    --  C122    ..     0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F17    --  C123    ..     0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F18    --  C123    ..     0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C110   --  C111    ..     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C120   --  C121    ..     0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C120   --  C122    ..     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F57    --  C231    ..     0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F59    --  C232    ..     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F60    --  C232    ..     0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F61    --  C233    ..     0.15 Ang.
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Alert level G

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PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large..       0.11
PLAT343_ALERT_2_G Check sp?      Angle Range in Main Residue for ..       C11
PLAT343_ALERT_2_G Check sp?      Angle Range in Main Residue for ..       C12
PLAT343_ALERT_2_G Check sp?      Angle Range in Main Residue for ..       C24
PLAT343_ALERT_2_G Check sp?      Angle Range in Main Residue for ..       C25
PLAT343_ALERT_2_G Check sp?      Angle Range in Main Residue for ..       C37
PLAT343_ALERT_2_G Check sp?      Angle Range in Main Residue for ..       C50
PLAT343_ALERT_2_G Check sp?      Angle Range in Main Residue for ..       C51
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C45
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .   176.00 A**3
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 0 ALERT level A = In general: serious problem
 4 ALERT level B = Potentially serious problem
42 ALERT level C = Check and explain
10 ALERT level G = General alerts; check

 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
33 ALERT type 2 Indicator that the structure model may be wrong or deficient
 1 ALERT type 3 Indicator that the structure quality may be low
18 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 13/08/2009; check.def file version of 12/08/2009