checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: sw210

Bond precision: C-C = 0.0072 A Wavelength=1.54178

Cell: **a=19.3395(7)** **b=19.3395(7)** **c=11.4546(6)**
alpha=90 **beta=90** **gamma=120**
Temperature: **100 K**

	Calculated	Reported
Volume	3710.2(3)	3710.2(3)
Space group	P 3 1 c	P 3 1 c
Hall group	P 3 -2c	P 3 -2c
Moiety formula	C16 Al F36 O4, 3(C10 H15 Fe P5), Ga	C16 Al F36 O4, 3(C10 H15 Fe P5), Ga
Sum formula	C46 H45 Al F36 Fe3 Ga O4 P15	C46 H45 Al F36 Fe3 Ga O4 P15
Mr	2074.62	2074.62
Dx,g cm-3	1.857	1.857
Z	2	2
Mu (mm-1)	9.429	9.429
F000	2048.0	2048.0
F000’	2055.32	
h,k,lmax	22,22,13	22,22,13
Nref	2126[4233]	4207
Tmin,Tmax	0.699,0.775	0.303,0.775
Tmin’	0.045	

Correction method= MULTI-SCAN

Data completeness= 1.98/0.99 **Theta(max)= 65.040**

R(reflections)= 0.0346(3696) **wR2(reflections)= 0.0862(4207)**

S = 1.019 **Npar= 319**

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
PLAT307_ALERT_2_A Isolated Metal Atom (Unusual !) Ga1

Author Response: There are coordinative Ga-P bonds with rather large Ga-P distances. These are neither taken into accout by the Platon cif generation module, nor by the checkCIF routine.

Alert level B

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PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for         O2
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for        Al1
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Alert level C

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THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5880
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C15
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C16
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ...         7
PLAT328_ALERT_4_C Check for Possibly Missing H on sp3? Phosphorus.         P1
PLAT328_ALERT_4_C Check for Possibly Missing H on sp3? Phosphorus.         P2
PLAT328_ALERT_4_C Check for Possibly Missing H on sp3? Phosphorus.         P3
PLAT328_ALERT_4_C Check for Possibly Missing H on sp3? Phosphorus.         P4
PLAT328_ALERT_4_C Check for Possibly Missing H on sp3? Phosphorus.         P5
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety         C6
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety         C7
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety         C8
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety         C9
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety        C10
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Alert level G

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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           65.04
          From the CIF: _reflns_number_total               4207
          Count of symmetry unique reflns          2126
          Completeness (_total/calc)            197.88%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured       2081
          Fraction of Friedel pairs measured      0.979
          Are heavy atom types Z>Si present          yes
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   1 ALERT level A = In general: serious problem
   2 ALERT level B = Potentially serious problem
  14 ALERT level C = Check and explain
   1 ALERT level G = General alerts; check

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 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
  11 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 25/02/2009; check.def file version of 25/02/2009

Datablock sw210 - ellipsoid plot