checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: compound_4

Bond precision: C-C = 0.0116 A   Wavelength=0.71073

Cell: a=18.0680(2)   b=19.9530(4)   c=25.3600(5)
                   alpha=90   beta=90   gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	9142.6(3)	9142.6(3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	?
Moiety formula	C48 H46 Ir O2 P2, F6 P, C H2 Cl2	C48 H46 Ir O2 P2, F6 P, C H2 Cl2
Sum formula	C49 H48 Cl2 F6 Ir O2 P3	C49 H48 Cl2 F6 Ir O2 P3
Mr	1138.90	1138.88
Dx,g cm-3	1.655	1.655
Z	8	8
Mu (mm-1)	3.207	3.207
F000	4544.0	4544.0
F000'	4539.33	
h,k,lmax	22,24,31	22,24,31
Nref	8995	8894
Tmin,Tmax	0.742,0.938	0.612,0.858
Tmin'	0.521	

Correction method= MULTI-SCAN

Data completeness= 0.989   Theta(max)= 26.000

R(reflections)= 0.0772(6903)   wR2(reflections)= 0.1040(8894)

S = 1.233   Npar= 533

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 C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given    0.158
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 .........   0.158 Report
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range      3.4 Ratio
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.0116 Ang.
PLAT350_ALERT_3_C Short   C-H (X0.96,N1.08A) C33    -   H33A   ...     0.78 Ang.
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Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF    Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.    55.12 Why ?
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.        1 Note
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =        3
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ir1    -- C45    ..      6.0 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ir1    -- C46    ..      5.7 su
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of       P3 Check
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL    2014 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: compound_5

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Bond precision:   C-C = 0.0105 A          Wavelength=0.71073

Cell:          a=43.3764(18)    b=10.0952(3)       c=22.0750(8)
               alpha=90         beta=105.089(2)    gamma=90
Temperature:   173 K
```

	Calculated	Reported
Volume	9333.2(6)	9333.2(6)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	?
Moiety formula	C48 H45 Ir O2 P2, C7 H8	C48 H45 Ir O2 P2, C7 H8
Sum formula	C55 H53 Ir O2 P2	C55 H53 Ir O2 P2
Mr	1000.13	1000.11
Dx,g cm-3	1.423	1.423
Z	8	8
Mu (mm-1)	2.970	2.970
F000	4048.0	4048.0
F000'	4039.47	
h,k,lmax	55,12,28	55,12,28
Nref	10287	10212
Tmin,Tmax	0.707,0.743	0.723,0.755
Tmin'	0.634	

Correction method= MULTI-SCAN

Data completeness= 0.993   Theta(max)= 27.100

R(reflections)= 0.0509(5727)   wR2(reflections)= 0.1148(10212)

S = 0.928   Npar= 541

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 C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.14 Report
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of   C55 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of   C50 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.5 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.0105 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H30   .. H42   ..   1.91 Ang.

⚪ Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF   Please Do !
PLAT128_ALERT_4_G Alternate Setting for Input Space Group   C2/c   I2/a Note
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .   166 A**3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #   2 Note
         C7 H8
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed   ! Info
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL   2014 Note

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```
0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
7 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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 20/08/2014; check.def file version of 18/08/2014