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: Minamida-324

Bond precision: C-C = 0.0047 A Wavelength=0.71075

Cell: a=11.0273(2) b=11.0909(2) c=24.6577(5)
alpha=89.4482(7) beta=80.5256(7) gamma=65.6118(7)
Temperature: 123 K

	Calculated	Reported
Volume	2703.42(9)	2703.42(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H20 Cl2 F42 P2 Pt	C44 H20 Cl2 F42 P2 Pt
Sum formula	C44 H20 Cl2 F42 P2 Pt	C44 H20 Cl2 F42 P2 Pt
Mr	1674.52	1674.52
Dx,g cm-3	2.057	2.057
Z	2	2
Mu (mm-1)	2.934	2.923
F000	1608.0	1608.0
F000’	1607.21	
h,k,lmax	14,14,32	14,14,32
Nref	12405	12385
Tmin,Tmax	0.711,0.943	0.779,0.943
Tmin’	0.658	

Correction method= # Reported T Limits: Tmin=0.779 Tmax=0.943
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.480

R(reflections)= 0.0312(11843) wR2(reflections)= 0.0886(12385)

S = 1.158 Npar= 820

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

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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       3.84 Report
PLAT213_ALERT_2_C Atom F40             has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom F42             has ADP max/min Ratio .....        3.3 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range        3.4 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1   F   Ueq(max)/Ueq(min) Range        6.0 Ratio
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Alert level G

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CHEMS02_ALERT_1_G  Please check that you have entered the correct
           _publ_requested_category classification of your compound;
           FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
           FO or CO or EO for organic.
           From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or
           From the CIF: _chemical_formula_sum:C44 H20 Cl2 F42 P2 Pt1
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.0007 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pt1    --  Cl1     ..        9.5 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C32 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F3     ..  F42     ..       2.84 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F7     ..  F36     ..       2.79 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F15    ..  F15     ..       2.82 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F16    ..  F33     ..       2.81 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F20    ..  F37     ..       2.81 Ang.
PLAT882_ALERT_1_G Missing datum for _diffrn_reflns_av_unetI/netI .     Please Check
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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
  12 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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* or *IUCrData*, 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 24/11/2016; check.def file version of 23/11/2016

Datablock Minamida-324 - ellipsoid plot