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: nz01r

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Bond precision:  C-C = 0.0103 A          Wavelength=0.71073

Cell:            a=15.4381(4)    b=33.2292(13)      c=31.2137(9)
                 alpha=90        beta=93.349(2)     gamma=90
Temperature:     150 K
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	Calculated	Reported
Volume	15985.2(9)	15985.1(9)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C155 H136 Cu3 P10 Ru2, F6 P, C1.50 H3 O0.50, 3.5(C3 H6 O)	?
Sum formula	C167 H160 Cu3 F6 O4 P11 Ru2	C167 H160 Cu3 F6 O4 P11 Ru2
Mr	3078.42	3078.37
Dx,g cm-3	1.279	1.279
Z	4	4
Mu (mm-1)	0.745	0.745
F000	6352.0	6352.0
F000’	6352.28	
h,k,lmax	20,44,41	19,43,41
Nref	40239	34429
Tmin,Tmax	0.875,0.942	0.877,1.000
Tmin’	0.862	

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Correction method= # Reported T Limits: Tmin=0.877 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.856          Theta(max)= 28.430

R(reflections)= 0.0768( 22179)    wR2(reflections)= 0.2185( 34429)

S = 1.076                 Npar= 1719
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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

PLAT234_ALERT_4_A Large Hirshfeld Difference P200 -- F201 .. 0.37 Ang.

Author Response: This refers to a PF6 anion in the structure that shows large thermal displacement/disorder. Splitting these atoms did not produce a model that could be refined.

PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 231 Ang3

Author Response: The structure crystallises as an acetone solvate with significant numbers of solvate molecules identified in the structure. The remaining voids presumably contain further disordered acetone solvate molecules which could not be modelled.

Alert level B

PLAT234_ALERT_4_B Large Hirshfeld Difference P200 -- F203 .. 0.30 Ang.

Author Response: This refers to a PF6 anion in the structure that shows large thermal displacement/disorder. Splitting these atoms did not produce a model that could be refined.

PLAT413_ALERT_2_B Short Inter XH3 .. XHn H23O .. H41 .. 1.91 Ang.

Alert level C

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 8
PLAT214_ALERT_2_C Atom F201 (Anion/Solvent) ADP max/min Ratio 4.1 prolat
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) ... 4.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C160 -- C161 .. 0.17 Ang.

Author Response: This refers to a PF6 anion in the structure that shows large thermal displacement/disorder. Splitting these atoms did not produce a model that could be refined.

PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C138 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C161 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.5 Note
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..... O229 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0103 Ang.
PLAT373_ALERT_2_C Long C(sp)-C(sp) Bond C2 - C3 ... 1.38 Ang.
PLAT373_ALERT_2_C Long C(sp)-C(sp) Bond C6 - C7 ... 1.37 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact H52B .. H161 .. 2.12 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H21F .. H63 .. 2.11 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H21I .. H106 .. 2.02 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 22 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 1 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 81.04 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 18 Report
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P200 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O217 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C216 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C217 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C214 is Constrained at 0.250 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C215 is Constrained at 0.250 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21M is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21N is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21O is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H21J is Constrained at 0.250 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H21K is Constrained at 0.250 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H21L is Constrained at 0.250 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H21X is Constrained at 0.250 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H21Y is Constrained at 0.250 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H21Z is Constrained at 0.250 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O213 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C210 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C211 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C212 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21D is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21E is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21F is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21G is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21H is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21I is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >O221 is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C218 is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C219 is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C220 is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H21P is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H21Q is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H21R is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H22D is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H22E is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H22F is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O225 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C222 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C223 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C224 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H22G is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H22H is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H22I is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H22J is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H22K is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H22L is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >O229 is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C226 is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C227 is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C228 is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H22M is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H22N is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H22O is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H22P is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H22Q is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H22R is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O233 is Constrained at 0.500 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of *C230   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C231   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C232   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23D   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23E   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23F   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23G   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23H   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23I   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O237   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C234   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C235   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C236   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23J   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23K   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23L   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23M   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23N   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23O   is Constrained at      0.500 Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =         70 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   7.50) in Resd. #          5 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   7.50) in Resd. #          7 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C4     Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C5     Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C26    Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C27    Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C137   Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C138   Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C25 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C217 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C210 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C212 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C218 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C220 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C222 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C224 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C226 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C228 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C230 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C232 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F203   ..  C210    ..      2.68 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F203   ..  C212    ..      2.72 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O237   ..  C214    ..      2.99 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
             C3 H6 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
             C3 H6 O
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        20 Note
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  15 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 106 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  25 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
  96 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

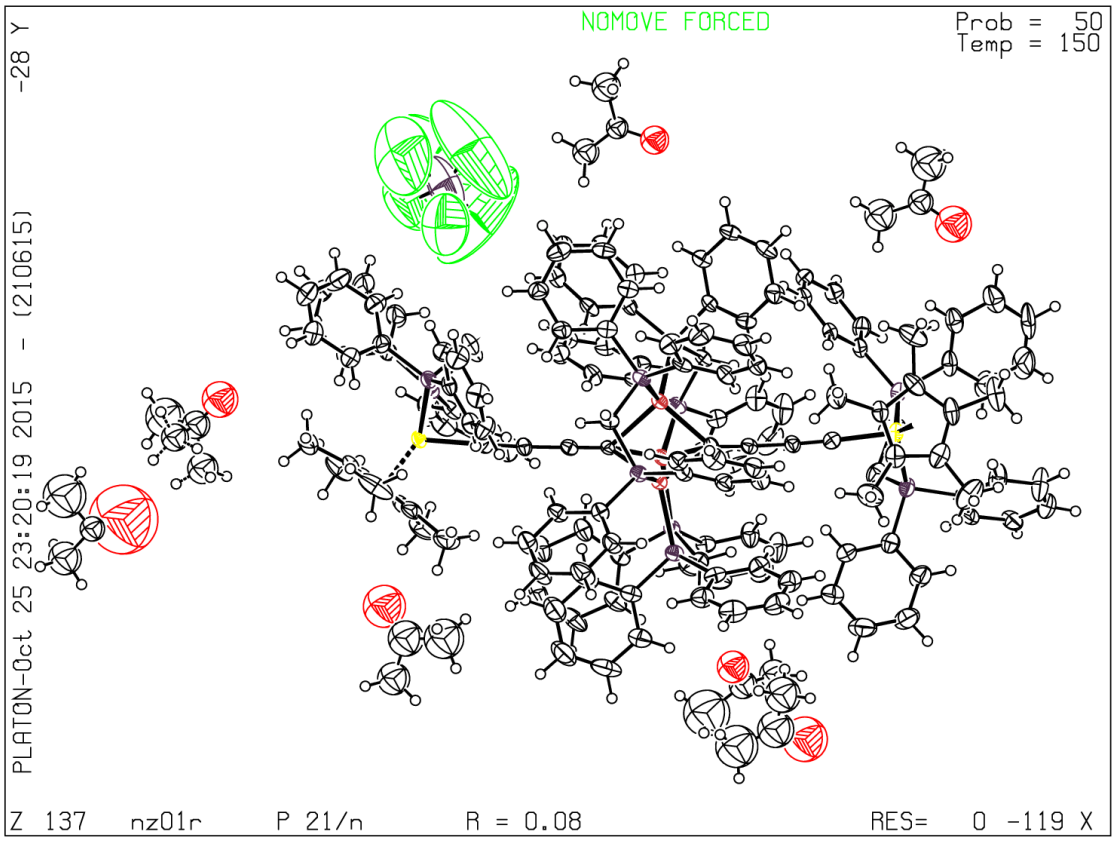
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 21/06/2015; check.def file version of 21/06/2015

Datablock nz01r - ellipsoid plot