checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: makino13

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Bond precision:  C-C = 0.0189 A          Wavelength=0.71073

Cell:             a=12.914(4)     b=13.120(4)     c=39.995(13)
                  alpha=90        beta=90         gamma=90
Temperature:      120 K
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	Calculated	Reported
Volume	6776(4)	6776(4)
Space group	I 21 21 21	I 21 21 21
Hall group	I 2b 2c	?
Moiety formula	C46 H42 N13 Ru2, 3(F6 P)	?
Sum formula	C46 H42 F18 N13 P3 Ru2	C46 H42 F18 N13 P3 Ru2
Mr	1413.98	1413.98
Dx,g cm-3	1.386	1.386
Z	4	4
Mu (mm-1)	0.605	0.605
F000	2816.0	2816.0
F000’	2808.79	
h,k,lmax	16,16,49	16,16,49
Nref	3834[6926]	6864
Tmin,Tmax	0.917,0.976	0.909,0.976
Tmin’	0.908	

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Correction method= MULTI-SCAN

Data completeness= 1.79/0.99      Theta(max)= 26.330

R(reflections)= 0.0988( 5222)     wR2(reflections)= 0.2594( 6864)

S = 1.039                 Npar= 372
```

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

PLAT231_ALERT_4_B Hirshfeld Test (Solvent)	P3	--	F7	..	11.8 su
PLAT234_ALERT_4_B Large Hirshfeld Difference	P2	--	F6	..	0.26 Ang.

Alert level C

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RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
           Weighted R factor given   0.259
PLAT084_ALERT_2_C High wR2 Value ..............................       0.26
PLAT214_ALERT_2_C Atom F6      (Anion/Solvent) ADP max/min Ratio         4.2 prola
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N5     --  C23     ..        5.5 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C20    --  C21     ..        5.3 su
PLAT234_ALERT_4_C Large Hirshfeld Difference N2     --  C6      ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N3     --  C7      ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N4     --  C13     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N6     --  N7      ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1     --  C2      ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C2     --  C3      ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C12    --  C13     ..       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C15    --  C16     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21    --  C22     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1     --  F1      ..       0.16 Ang.
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         N6
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C7
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C9
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C12
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C16
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C18
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C8
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C17
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of          P1
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of          P2
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of          P3
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0189 Ang
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C1     -   C2     ...       1.40 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C12    -   C13    ...       1.40 Ang.
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....          9
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.13
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      54.74
PLAT104_ALERT_1_G The Reported Crystal System is Inconsistent with   I212121
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   P3     --  F8      ..        8.6 su
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   P3     --  F9      ..        6.8 su
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          5
           N6  -RU1 -N1  -C18   -98.00  8.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         10
           N6  -RU1 -N1  -C1     20.00  8.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         15
           N6  -RU1 -N1  -C12   143.00  8.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         57
           N1  -RU1 -N6  -N7    -69.00  9.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         61
           RU1 -N6  -N7  -N6   -160.80  1.40   1.555   1.555   1.555   2.655
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4
             F6 P
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         54
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  2 ALERT level B = A potentially serious problem, consider carefully
 29 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 19 ALERT level G = General information/check it is not something unexpected

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 17 ALERT type 2 Indicator that the structure model may be wrong or deficient
  3 ALERT type 3 Indicator that the structure quality may be low
 25 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*, 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 05/11/2012; check.def file version of 05/11/2012

Datablock makino13 - ellipsoid plot