

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: makino17

Bond precision: C-C = 0.0060 Å

Wavelength=0.71073

Cell: a=13.4461(13) b=14.5506(14) c=16.7938(16)
 alpha=73.877(1) beta=89.452(1) gamma=84.856(1)
Temperature: 120 K

	Calculated	Reported
Volume	3143.3(5)	3143.3(5)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C23 H21 N8 Ru, F6 P	?
Sum formula	C23 H21 F6 N8 P Ru	C23 H21 F6 N8 P Ru
Mr	655.52	655.52
Dx,g cm-3	1.385	1.385
Z	4	4
Mu (mm-1)	0.610	0.610
F000	1312.0	1312.0
F000'	1308.00	
h,k,lmax	17,18,21	17,18,21
Nref	14588	13576
Tmin,Tmax	0.916,0.958	0.872,0.959
Tmin'	0.869	

Correction method= MULTI-SCAN

Data completeness= 0.931

Theta(max)= 27.600

R(reflections)= 0.0464(10000)

wR2(reflections)= 0.1147(13576)

S = 1.034

Npar= 721

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low 0.930

Alert level B



Alert level C

PLAT220_ALERT_2_C Large Non-Solvent N Ueq(max)/Ueq(min) ... 3.9 Ratio
 PLAT230_ALERT_2_C Hirshfeld Test Diff for N6 -- N7 .. 6.7 su
 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 P1



Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites 2
 PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ?
 PLAT104_ALERT_1_G The Reported Crystal System is Inconsistent with P-1
 PLAT154_ALERT_1_G The su's on the Cell Angles are Equal 0.00100 Deg.
 PLAT194_ALERT_1_G Missing _cell_measurement_reflms_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) P2 -- F10 .. 8.7 su
 PLAT302_ALERT_4_G Note: Anion/Solvent Disorder 14 Perc.
 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 -C12 -51.00 4.00 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 70.00 4.00 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 -C18 -171.00 4.00 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 56
 N1 -RU1 -N6 -N7 -161.00 4.00 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 -N8 170.00 7.00 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 66
 N14 -RU2 -N9 -C41 5.00 3.00 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 71
 N14 -RU2 -N9 -C35 126.00 3.00 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 76
 N14 -RU2 -N9 -C24 -115.00 3.00 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 117
 N9 -RU2 -N14 -N15 171.00 3.00 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 122
 RU2 -N14 -N15 -N16 -152.00 7.00 1.555 1.555 1.555 1.555
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 64
 F13 -P2 -F9 1.555 1.555 1.555 21.40 Deg.
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 67
 F14 -P2 -F10 1.555 1.555 1.555 13.70 Deg.
 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 12
 PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed !

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 25 **ALERT level G** = General information/check it is not something unexpected
- 5 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
 2 ALERT type 3 Indicator that the structure quality may be low
 19 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.

