checkCIF/PLATON report

Structure factors have been supplied for datablock(s) paul017

No syntax errors found. CIF dictionary Interpreting this report

Datablock: paul017

Bond precision: C-C = 0.0044 A Wavelength=0.71073

Cell: a=15.6613(14) b=16.8213(16) c=19.0713(17)
alpha=107.424(4) beta=100.597(4) gamma=105.364(4)
Temperature: 110 K

	Calculated	Reported
Volume	4429.1(7)	4429.1(7)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	4(C30 H24 N6 O2 Ru), C7 H5 N, 8(F6 P), 8(C4 H10 O)	?
Sum formula	C159 H181 F48 N25 O16 P8 Ru4	C79.50 H90.50 F24 N12.50 O8 P4 Ru2
Mr	4262.33	2131.16
Dx,g cm-3	1.598	1.598
Z	1	2
Mu (mm-1)	0.525	0.525
F000	2166.0	2166.0
F000’	2163.12	
h,k,lmax	24,25,29	24,25,29
Nref	33910	33738
Tmin,Tmax	0.934,0.959	0.935,0.959
Tmin’	0.934	

Correction method= MULTI-SCAN

Data completeness= 0.995 Theta(max)= 33.190

R(reflections)= 0.0551(20396) wR2(reflections)= 0.1482(33738)

S = 1.019 Npar= 1303

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
PLAT973_ALERT_2_B Large Calcd. Positive Residual Density on Ru2 1.86 eA-3

Alert level C

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PLAT045_ALERT_1_C Calculated and Reported Z Differ by .....        0.50 Ratio
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
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of     P4
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....    2.1
PLAT354_ALERT_3_C Short   O-H Bond (0.82A)   O1     -   H1     ...   0.67 Ang.
PLAT354_ALERT_3_C Short   O-H Bond (0.82A)   O4     -   H4     ...   0.66 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #      1
             C30 H24 N6 O2 Ru
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) .....     2
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600     3
PLAT912_ALERT_4_C Missing # of FCF Reflections Above STh/L=  0.600   161
PLAT971_ALERT_2_C Large Calcd. Non-Metal Positive Residual Density   1.68 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite     20
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....     20
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....      ?
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .........  0.00400 Deg.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ru1    --  N5      ..    5.2 su
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of     C66
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..................     27 Perc.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......   282
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
13 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
8 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 19/04/2012; check.def file version of 14/04/2012

Datablock paul017 - ellipsoid plot