checkCIF/PLATON report

Structure factors have been supplied for datablock(s) paul020s

No syntax errors found. CIF dictionary Interpreting this report

Datablock: paul020s

```
Bond precision:  C-C = 0.0031 A          Wavelength=0.71073

Cell:          a=9.4108(7)       b=12.2807(9)     c=13.0032(10)
               alpha=84.343(4)   beta=88.748(4)   gamma=73.877(4)
Temperature:   120 K
```

	Calculated	Reported
Volume	1436.63(19)	1436.63(19)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C30 H22 N6 O2 Ru	?
Sum formula	C30 H22 N6 O2 Ru	C33 H28.50 N6.50 O2.50 Ru
Mr	599.61	657.19
Dx,g cm-3	1.386	1.519
Z	2	2
Mu (mm-1)	0.582	0.591
F000	608.0	672.0
F000’	605.67	
h,k,lmax	13,18,19	13,18,19
Nref	9795	9615
Tmin,Tmax	0.899,0.943	0.901,0.943
Tmin’	0.899	

```
Correction method= MULTI-SCAN

Data completeness= 0.982          Theta(max)= 31.790

R(reflections)= 0.0368( 7918)     wR2(reflections)= 0.0889( 9615)

S = 1.024                 Npar= 352
```

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

CHEMW03_ALERT_2_B WARNING: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.95 <> 1.05

From the CIF: _cell_formula_units_Z 2

```
From the CIF: _chemical_formula_weight          657.19
TEST: Calculate formula weight from _atom_site_*
atom     mass    num     sum
C        12.01   30.00  360.33
H         1.01   22.00   22.18
N        14.01    6.00   84.04
O        16.00    2.00   32.00
Ru      101.07    1.00  101.07
Calculated formula weight             599.62
```

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C2     --  C3      ..        6.5 su
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          2
PLAT975_ALERT_2_C Positive Residual Density at 0.83A from O1     .       0.52 eA-3
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C33 H28.5 N6.5 O2.5 Ru1
           Atom count from the _atom_site data:  C30 H22 N6 O2 Ru1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C33 H28.50 N6.50 O2.50 Ru
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         66.00     60.00    6.00
           H         57.00     44.00   13.00
           N         13.00     12.00    1.00
           O          5.00      4.00    1.00
           Ru         2.00      2.00    0.00
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    --  N4      ..        5.4 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ru1    --  N5      ..        5.3 su
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .        277 A**3
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        182
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......          !
```

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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
  5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 11 ALERT level G = General information/check it is not something unexpected

  5 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
  1 ALERT type 3 Indicator that the structure quality may be low
  3 ALERT type 4 Improvement, methodology, query or suggestion
  2 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 04/07/2012; check.def file version of 28/06/2012

Datablock paul020s - ellipsoid plot