checkCIF/PLATON report

Structure factors have been supplied for datablock(s) igrum

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: igrum

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Bond precision:   C-C = 0.0057 A          Wavelength=0.71073

Cell:           a=10.560(2)         b=20.205(4)        c=22.352(4)
                alpha=114.814(4)    beta=101.570(4)    gamma=90.753(4)
Temperature:    120 K

                 Calculated                 Reported
Volume           4215.4(14)                 4215.4(14)
Space group      P -1                       P -1
Hall group       -P 1                       -P 1
Moiety formula   C44 H45 B8 Cl O P2 Ru2     ?
Sum formula      C44 H45 B8 Cl O P2 Ru2     C44 H45 B8 Cl O P2 Ru2
Mr               975.81                     975.81
Dx,g cm-3        1.538                      1.538
Z                4                          4
Mu (mm-1)        0.892                      0.892
F000             1968.0                     1968.0
F000'            1959.78
h,k,lmax         14,27,30                   14,27,30
Nref             22432                      22374
Tmin,Tmax        0.717,0.852                0.659,0.862
Tmin'            0.657

Correction method= # Reported T Limits: Tmin=0.659 Tmax=0.862
AbsCorr = MULTI-SCAN

Data completeness= 0.997           Theta(max)= 29.000

R(reflections)= 0.0462( 15232)                wR2(reflections)=
                                              0.1000( 22374)
S = 1.075                  Npar= 1102
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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 C

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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.79 Report
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        8.0 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2  H   Uiso(max)/Uiso(min) Range        4.6 Ratio
PLAT245_ALERT_2_C U(iso) H3A       Smaller than U(eq) B3A       by      0.014 Ang**2
PLAT245_ALERT_2_C U(iso) H4A       Smaller than U(eq) B4A       by      0.017 Ang**2
PLAT245_ALERT_2_C U(iso) H10B      Smaller than U(eq) B10B      by      0.014 Ang**2
PLAT330_ALERT_2_C Large Aver Phenyl C-C Dist C18A     --C23A     .       1.41 Ang.
PLAT330_ALERT_2_C Large Aver Phenyl C-C Dist C18B     --C23B     .       1.42 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.188 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.87Ang From Ru2A            1.57 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Ru1A       1.42 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Ru1B       1.41 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Ru2A       1.37 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Ru2B       1.36 eA-3
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Alert level G

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PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.004 Degree
PLAT303_ALERT_2_G Full Occupancy Atom H5A       with # Connections       2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H9A       with # Connections       2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H5B       with # Connections       2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H9B       with # Connections       2.00 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for        C1A Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for        C1B Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      42.00 Deg.
              RU1B -B9B  -H9B     1_555   1_555   1_555 ......     #  627 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         55 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.4 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       58.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  20 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
   2 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* or *IUCrData*, 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 18/05/2022; check.def file version of 17/05/2022

Datablock igrum - ellipsoid plot