checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rhco

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: rhco

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Bond precision:  C-C = 0.0320 A          Wavelength=0.71073

Cell:            a=11.319(5)     b=15.288(7)          c=16.746(7)
                 alpha=90        beta=93.575(17)      gamma=90
Temperature:     296 K

                Calculated                Reported
Volume          2892(2)                   2892(2)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C26 H32 B2 Co2 O6 Rh2     ?
Sum formula     C26 H32 B2 Co2 O6 Rh2     C26 H32 B2 Co2 O6 Rh2
Mr              785.82                    785.81
Dx,g cm-3       1.805                     1.805
Z               4                         4
Mu (mm-1)       2.286                     2.286
F000            1560.0                    1560.0
F000'           1554.31
h,k,lmax        13,18,19                  13,18,19
Nref            5094                      4825
Tmin,Tmax       0.727,0.796               0.684,0.804
Tmin'           0.656

Correction method= # Reported T Limits: Tmin=0.684 Tmax=0.804
AbsCorr = MULTI-SCAN

Data completeness= 0.947          Theta(max)= 24.994

R(reflections)= 0.1152( 2452)     wR2(reflections)= 0.3501( 4825)

S = 1.033                  Npar= 354
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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 A

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Rh1 2.09 eA-3

Author Response: The alert was mainly due to there is q peak that not assigned to any element. However, when observed closely the electron density appears to be around Cp* ring and also near to the metal centres. Thus,such residual density is likely not from unaccounted atom types.

Alert level B

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low . 0.947 Why?

Author Response: : Even though crystal data was attempted to collected up to 0.78 \%A resolution, the crystal (the largest available) still diffracted quite weakly at high angle.

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.032 Ang.

Author Response: C-C bonds in Cp* is somewhat mobile, low temperature measurement could have averted this alarm.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.15A From Rh2 3.11 eA-3

Author Response: The alert was mainly due to there is q peak that not assigned to any element. However, when observed closely the electron density appears to be around Cp* ring and also near to the metal centres. Thus,such residual density is likely not from unaccounted atom types.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.17A From Rh1 2.57 eA-3

Author Response: The alert was mainly due to there is q peak that not assigned to any element. However, when observed closely the electron density appears to be around Cp* ring and also near to the metal centres. Thus,such residual density is likely not from unaccounted atom types.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.145
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.145 Report
PLAT082_ALERT_2_C High R1 Value ..... 0.12 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.35 Report
PLAT213_ALERT_2_C Atom B1 has ADP max/min Ratio ..... 3.1 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference Rh1 --C5 . 0.20 Ang.

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PLAT234_ALERT_4_C Large Hirshfeld Difference Rh2      --B1       .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Co1      --C21      .       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11      --C15      .       0.24 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Rh1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C22 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.594        269 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.18A   From Rh1             2.42 eA-3
```

Author Response: The alert was mainly due to there is q peak that not assigned to any element. However, when observed closely the electron density appears to be around Cp* ring and also near to the metal centres. Thus,such residual density is likely not from unaccounted atom types.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.13A   From Rh2             2.36 eA-3
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Author Response: The alert was mainly due to there is q peak that not assigned to any element. However, when observed closely the electron density appears to be around Cp* ring and also near to the metal centres. Thus,such residual density is likely not from unaccounted atom types.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.21A   From Rh2             2.23 eA-3
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Author Response: The alert was mainly due to there is q peak that not assigned to any element. However, when observed closely the electron density appears to be around Cp* ring and also near to the metal centres. Thus,such residual density is likely not from unaccounted atom types.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.16A   From Rh2             1.87 eA-3
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Author Response: The alert was mainly due to there is q peak that not assigned to any element. However, when observed closely the electron density appears to be around Cp* ring and also near to the metal centres. Thus,such residual density is likely not from unaccounted atom types.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.96A   From C13             1.71 eA-3
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Author Response: The alert was mainly due to there is q peak that not assigned to any element. However, when observed closely the electron density appears to be around Cp* ring and also near to the metal centres. Thus,such residual density is likely not from unaccounted atom types.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.06A   From B1              1.54 eA-3
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Author Response: The alert was mainly due to there is q peak that not assigned to any element. However, when observed closely the electron density appears to be around Cp* ring and also near to the metal centres. Thus,such residual density is likely not from unaccounted atom types.

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.83A   From Rh1            -2.26 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.90A   From Rh2            -2.06 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.91A   From Rh1            -1.97 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.98A   From Rh2            -1.85 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.94A   From Rh2            -1.73 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H16C             -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H19B             -0.55 eA-3
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Alert level G

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PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C25 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........        3.8 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  26 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   6 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  24 ALERT type 2 Indicator that the structure model may be wrong or deficient
   8 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 05/12/2020; check.def file version of 05/12/2020

Datablock rhco - ellipsoid plot