checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Muraoka6

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: Muraoka6

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Bond precision:   C-C = 0.0040 A              Wavelength=1.54187

Cell:          a=8.83401(16)      b=12.5026(2)      c=18.7047(3)
               alpha=103.5820(9)  beta=94.5117(9)  gamma=103.4930(9)
Temperature:  153 K

                  Calculated                    Reported
Volume            1933.14(6)                    1933.14(6)
Space group       P -1                          P -1
Hall group        -P 1                          -P 1
                  C28 H30 N2 O6, C14 H12 N2, C28 H30 N2 O6, C14 H12 N2,
Moiety formula
                  0.5(C4 H8 O2), H2 O           0.5(C4 H8 O2), H2 O
Sum formula       C44 H48 N4 O8                 C44 H48 N4 O8
Mr                760.86                        760.89
Dx,g cm-3         1.307                         1.307
Z                 2                             2
Mu (mm-1)         0.736                         0.737
F000              808.0                         808.0
F000'             810.50
h,k,lmax          10,15,22                      10,15,22
Nref              7077                          6848
Tmin,Tmax         0.838,0.863                   0.704,0.863
Tmin'             0.745

Correction method= # Reported T Limits: Tmin=0.704 Tmax=0.863
AbsCorr = MULTI-SCAN

Data completeness= 0.968          Theta(max)= 68.230

R(reflections)= 0.0504( 4378)      wR2(reflections)= 0.1459( 6848)

S = 1.061                   Npar= 515
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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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PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.970 Why?
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00405 Ang.
PLAT355_ALERT_3_C Long    O-H (X0.82,N0.98A)  O8        - H6       .      1.03 Ang.
PLAT355_ALERT_3_C Long    O-H (X0.82,N0.98A)  O8        - H7       .      1.04 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.948 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=     0.600        208 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....          1 Check
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
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⚪ Alert level G

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CHEMS02_ALERT_1_G  Please check that you have entered the correct
             _publ_requested_category classification of your compound;
             FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
             FO or CO or EO for organic.
             From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or A
             From the CIF: _chemical_formula_sum :C44 H48 N4 O8
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       3 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............       2 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)  0.0009 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       2 Report
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O7         109.7 Degree
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       4 Note
             H2 O
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       2 Note
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......  Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      20 Note
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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
   8 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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
   3 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 03/05/2019; check.def file version of 29/04/2019

NOMOVE FORCED

Prob = 50
Temp = 153

42 Y

PLATON-Jul 11 12:38:58 2019 - (70316)

Z 106   Muraoka6   P -1   R = 0.05   RES=   0   -24 X