checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: c313

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Bond precision:   C-C = 0.0088 A           Wavelength=0.71070

Cell:            a=35.837(2)     b=7.9677(5)          c=10.8502(7)
                 alpha=90        beta=99.028(9)       gamma=90
Temperature:     100 K

                 Calculated              Reported
Volume           3059.8(3)               3059.8(3)
Space group      C 2/c                   C2/c
Hall group       -C 2yc                  ?
Moiety formula   F6 O4.80 Re, 4(C10 H8 S8)  ?
Sum formula      C40 H32 F6 O4.80 Re S32    C40 H32 F6 O4.80 Re S32
Mr               1915.59                 1915.58
Dx,g cm-3        2.079                   2.079
Z                2                       2
Mu (mm-1)        3.142                   3.142
F000             1902.8                  1903.0
F000'            1909.25
h,k,lmax         44,9,13                 44,9,13
Nref             3032                    3028
Tmin,Tmax        0.475,0.730             0.318,1.000
Tmin'            0.451

Correction method= # Reported T Limits: Tmin=0.318 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999         Theta(max)= 26.070

R(reflections)= 0.0702( 2616)     wR2(reflections)= 0.1947( 3028)

S = 1.005                  Npar= 207
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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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PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..    Please Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.0088 Ang.
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        7 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        1 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF    Please Do !
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...    Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.10 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     59.58 Why ?
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as    mixed Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group     C2/c    I2/a Note
PLAT300_ALERT_4_G Atom Site Occupancy of Re1        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow1        Constrained at     0.72 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow2        Constrained at     0.48 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow3        Constrained at     0.24 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )    100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  1 )     5.90 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....     Ow2 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       3 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .    1.29 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      68 Check
         OW1  -F4   -OW3    1.555   1.555   1.555          36.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      69 Check
         OW1  -F4   -RE1    1.555   1.555   1.555          24.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      73 Check
         OW1  -F5   -OW2    1.555   1.555   1.555          33.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      75 Check
         OW1  -F5   -RE1    1.555   1.555   1.555          17.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      76 Check
         OW2  -F5   -RE1    1.555   1.555   1.555          25.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      77 Check
         OW2  -F2   -RE1    1.555   1.555   1.555          26.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      78 Check
         OW2  -F6   -RE1    1.555   1.555   1.555          20.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #     119 Check
         OW1  -OW2  -F5     1.555   1.555   1.555          43.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #     121 Check
         F6   -OW2  -F5     2.556   1.555   1.555          33.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #     128 Check
         OW1  -OW2  -F5     2.556   1.555   2.556          43.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #     130 Check
         F6   -OW2  -F5     1.555   1.555   2.556          33.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #     135 Check
         OW1  -OW3  -RE1    1.555   1.555   1.555          23.40 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #       9 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      18 Note
PLAT899_ALERT_4_G SHELXL97  is Deprecated and Succeeded by SHELXL/    2018 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
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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  38 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
  29 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 18/09/2020; check.def file version of 20/08/2020