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: 4777447447

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Bond precision:   I- O = 0.0152 A          Wavelength=0.71073

Cell:           a=30.02(4)     b=10.205(13)          c=7.762(10)
                alpha=90       beta=103.786(15)      gamma=90
Temperature:    296 K

                Calculated                 Reported
Volume          2309(5)                    2310(5)
Space group     C c                        Cc
Hall group      : C -2yc                   ?
Moiety formula  I8 Mo8 O48, 3.802(Rb),     ?
                4.198(K)
Sum formula     I8 K4.20 Mo8 O48 Rb3.80    I2 K Mo2 O12 Rb
Mr              3039.82                    762.25
Dx,g cm-3       4.372                      4.384
Z               2                          8
Mu (mm-1)       11.937                     12.122
F000            2728.9                     2736.0
F000'           2689.78
h,k,lmax        38,13,10                   38,13,9
Nref            5300[ 2653]                4475
Tmin,Tmax                                  0.575,0.746
Tmin'

Correction method= # Reported T Limits: Tmin=0.575 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.69/0.84      Theta(max)= 27.510

R(reflections)= 0.0534( 3907)     wR2(reflections)= 0.1195( 4475)

S = 1.049                 Npar= 327
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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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as multi-scan
STRVA01_ALERT_4_C   Flack test results are meaningless.
          From the CIF: _refine_ls_abs_structure_Flack   0.000
          From the CIF: _refine_ls_abs_structure_Flack_su   10.000
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .   0.977 Why?
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..   9.18 Check
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .   1.53 %
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...   Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...   Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...   Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..   Please Check
PLAT148_ALERT_3_C s.u. on the   a   - Axis is (Too) Large ....   0.040 Ang.
PLAT148_ALERT_3_C s.u. on the   b   - Axis is (Too) Large ....   0.0130 Ang.
PLAT148_ALERT_3_C s.u. on the   c   - Axis is (Too) Large ....   0.010 Ang.
PLAT213_ALERT_2_C Atom I4   has ADP max/min Ratio .....   3.6 prolat
PLAT213_ALERT_2_C Atom O5   has ADP max/min Ratio .....   3.1 prolat
PLAT213_ALERT_2_C Atom O8   has ADP max/min Ratio .....   3.4 prolat
PLAT213_ALERT_2_C Atom O10   has ADP max/min Ratio .....   3.1 prolat
PLAT213_ALERT_2_C Atom O22   has ADP max/min Ratio .....   3.6 prolat
PLAT213_ALERT_2_C Atom O23   has ADP max/min Ratio .....   3.8 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 I   Ueq(max)/Ueq(min) Range   3.9 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 O   Ueq(max)/Ueq(min) Range   4.6 Ratio
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   Mo3 Check

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⚪ 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:I2 K1 Mo2 O12 Rb1
           Atom count from the _atom_site data: I2 K1.0495 Mo2 O12 Rb0.9505
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   8
          From the CIF: _chemical_formula_sum I2 K Mo2 O12 Rb
          TEST: Compare cell contents of formula and atom_site data

          atom   Z*formula cif sites diff
          I   16.00   16.00   0.00
          K   8.00   8.40   -0.40
          Mo   16.00   16.00   0.00
          O   96.00   96.00   0.00
          Rb   8.00   7.60   0.40
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   3 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF   Please Do !
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .   10.000 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.25 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   47.36 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group Cc   Ia Note

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PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )        100% Note
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O24       125.4 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Mo1        (VI)    .    6.10 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mo2        (VI)    .    6.09 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mo3        (VI)    .    6.33 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mo4        (VI)    .    6.20 Info
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and s.u.   10.00 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............    20 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
 23 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 22 ALERT level G = General information/check it is not something unexpected

 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 13 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
 10 ALERT type 4 Improvement, methodology, query or suggestion
  6 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 26/09/2018; check.def file version of 13/09/2018