checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 11_cr3_a638nm_a

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.

Datablock: 11_cr3_a638nm_a

```
Bond precision:
                  N-C = 0.0159 A
                                            Wavelength=0.68890
Cell:
                a=9.0224(6)
                                   b=9.3760(5)
                                                     c=9.7105(9)
                                  beta=82.500(7)
                alpha = 87.576(6)
                                                    gamma = 70.809(5)
                30 K
Temperature:
                Calculated
                                             Reported
Volume
                769.16(10)
                                             769.16(10)
Space group
                P -1
                                            P -1
Hall group
                -P 1
                                             -P 1
                C7 Mo N7, 0.22(O2),
                                             C7 K4 Mo N7 O2
Moiety formula
                1.56(O), 4(K)
Sum formula
                C7 K4 Mo N7 O2
                                            C7 K4 Mo N7 O2
                466.48
                                             466.48
Dx,g cm-3
                2.014
                                             2.014
                2
                1.767
                                             1.757
Mu (mm-1)
F000
                450.0
                                             450.0
F000'
                447.80
h,k,lmax
                12,13,13
                                             12,13,13
Nref
                4534
                                             4066
Tmin, Tmax
                0.939,0.983
                                             0.999,1.000
Tmin'
                0.932
Correction method= # Reported T Limits: Tmin=0.999 Tmax=1.000
AbsCorr = EMPIRICAL
Data completeness= 0.897
                                    Theta (max) = 29.077
                                                       wR2 (reflections) =
R(reflections) = 0.1087(2499)
                                                       0.2703 (4066)
S = 1.047
                           Npar= 200
```

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.91Ang From Mo1A

6.56 eA-3

Author Response: This is due to slight fatigue of the crystal caused by light radiation

Alert level B

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density

8.24 eA-3

Author Response: This is due to slight fatigue of the crystal caused by light radiation

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 01A Check

Author Response: The water molecules in the structure are disordered, so we decided not model the positions of the hydrogen atoms, since the refinement led to an unphys

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.78Ang From K4A

2.70 eA-3

Author Response: This is due to slight fatigue of the crystal caused by light radiation

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.86Ang From K3A

2.61 eA-3

Author Response: This is due to slight fatigue of the crystal caused by light radiation

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on

Mo1A

1.63 eA-3

Author Response: This is due to slight fatigue of the crystal caused by light radiation


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PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range
                                                                     3.1 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range
                                                                    4.2 Ratio
                                                                 20.545 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....
                                                                  3.815 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600
                                                                      61 Report
               2 -6 5, 0 7 5, -1 -6 6, 0 -6 6,
                                                       1 -6 6, 6 5 6,
               1 -5 7,
                         2 -5 7,
                                  -4 1 7,
                                             6 1 7, -3 2 7, 6 2 7,
                       6 4 7, -3 1 8,
2 -1 9, 2 0 9,
               6 3 7,
1 -1 9,
                                            -2 2 8, -1 3 8, 2 -3 9,
-1 1 9, 0 2 9, 1 -3 10,
                                            3 -2 10,
               2 -3 10,
                                   2 -2 10,
                         1 -2 10,
                                                        0 -1 10,
                                                                   1 - 1 10.
                                   0 0 10,
                                             1 0 10,
               2 - 1 10,
                         3 -1 10,
                                                        2 0 10,
                                                                   3 0 10,
                                             4 1 10,
               4 0 10,
                         2 1 10,
                                   3 1 10,
                                                        0 -3 11,
                                                                   1 -3 11,
               0 -2 11,
                                   2 -2 11,
                        1 -2 11,
                                              3 -2 11,
                                                        0 -1 11,
                                                                   1 -1 11,
                        3 -1 11,
                                   0 0 11,
               2 -1 11,
                                             1 0 11,
                                                        2 0 11,
                                                                   3 0 11,
                        1 1 11,
               4 0 11,
                                   2 1 11,
                                            3 1 11,
                                                        4 1 11,
                                                                   3 2 11,
               4 2 11,
                                                                   1.67 eA-3
PLAT925_ALERT_1_C The Reported and Calculated Rho(max) Differ by .
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.83Ang From K1A
                                                                     2.28 eA-3
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Author Response: This is due to slight fatigue of the crystal caused by light radiation

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.80Ang From K2A 1.72 eA-3

Author Response: This is due to slight fatigue of the crystal caused by light radiation

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From Mo1A -2.48 eA-3 PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.82Ang From N1A . 0.79 eA-3

Alert level G

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\verb|ABSMU01_ALERT_1_G| Calculation of \verb|_exptl_absorpt_correction_mu| \\
               not performed for this radiation type.
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms
                                                                          4 Report
                                                                   Please Check
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..
                                                                    23.45 Why ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records
                                                                          3 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)
                                                                      100% Note
PLAT302 ALERT 4 G Anion/Solvent/Minor-Residue Disorder (Resd 4)
                                                                      100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2)
                                                                      0.88 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 4)
                                                                      0.56 Check
                                                                      02A Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #
                                                                         3 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #
                                                                          4 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #
                                                                          5 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #
                                                                          6 Note
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters
                                                                          8 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
                                                                        24 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..
                                                                   Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).
                                                                         1 Note
               0 0 1,
```

8 ALERT type 3 Indicator that the structure quality may be low 11 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

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.

