checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 7_cr2_a405nm_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.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 7_cr2_a405nm_a

Bond precision: N- C = 0.0097 A Wavelength=0.68890

Cell:	a=9.6002(9)	b=9.6496(11)	c=9.7097(8)
	alpha=65.687(9)	beta=87.767(8)	gamma=88.774(10)
Temperature:	30 K		

	Calculated	Reported
Volume	819.08(15)	819.08(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C6 Mo N6, C N, 2(O), 4(K)	C7 K3.779 Mo N7 O2, 0.221(K)
Sum formula	C7 K4 Mo N7 O2	C7 K4 Mo N7 O2
Mr	466.48	466.48
Dx,g cm-3	1.891	1.891
Z	2	2
Mu (mm-1)	1.660	1.650
F000	450.0	450.0
F000'	447.80	
h,k,lmax	12,12,12	12,12,12
Nref	4056	3915
Tmin,Tmax	0.942,0.984	0.996,1.000
Tmin'	0.936	

Correction method= # Reported T Limits: Tmin=0.996 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.965 Theta(max)= 27.339

R(reflections)= 0.0621(2863) wR2(reflections)= 0.1679(3915)

S = 1.032 Npar= 199

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 B

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .... O1B Check

Author Response: An attempt to model the position of hydrogen atoms for the photoinduce state led to instability of the refinement.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .... O2B Check

Author Response: An attempt to model the position of hydrogen atoms for the photoinduce state led to instability of the refinement.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.45Ang From C3B 3.47 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. 0.92Ang From Mo1B 2.58 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. 1.38Ang From C5B 2.51 eA-3

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

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Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.976 Why?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C6 Mo N6, C N, 2(O), 4(K)
Rep.: C7 K3.779 Mo N7 O2, 0.221(K)
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.77 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 3.64 eA-3
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 70 Report

-11	3	0,	-10	4	0,	-9	4	0,	-10	5	0,	-9	5	0,	-8	5	0,
-9	6	0,	-8	6	0,	-8	7	0,	8	-7	1,	8	-6	1,	9	-6	1,
8	-5	1,	9	-5	1,	9	-4	1,	10	-4	1,	9	-3	1,	-9	0	1,
-10	4	1,	-9	4	1,	-10	5	1,	-9	5	1,	-8	5	1,	-7	5	1,
-9	6	1,	-8	6	1,	-7	6	1,	-8	7	1,	-7	7	1,	-7	8	1,
8	-6	2,	7	-5	2,	9	-5	2,	8	-4	2,	10	-4	2,	-9	1	2,
-9	2	2,	-9	3	2,	-9	4	2,	-10	5	2,	-9	5	2,	-9	6	2,
-8	6	2,	-9	7	2,	-8	7	2,	-8	8	2,	-4	8	2,	7	-4	3,

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               -8  0  3, -10  5  3,  -9  6  3,  -9  7  3,  -8  7  3,  -7  7  3,
               -8  8  3,  -5  8  3,  -4  8  3,   6 -4  4,   7 -3  4,  -6  7  4,
               -8  8  4,  -5  8  4,  -4  8  4,   4 -4  5,   5 -3  5,   6 -2  5,
               -4  8  5,  -3  8  6,  -2  8  6,   6  4  7,
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.01Ang From O1B     .       0.83 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.41Ang From O2B     .      -0.62 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.71Ang From O1B     .      -0.56 eA-3
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _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          2 Report
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0010 Report
PLAT300_ALERT_4_G Atom Site Occupancy of K1B        Constrained at     0.7786 Check
PLAT300_ALERT_4_G Atom Site Occupancy of K1C        Constrained at     0.2214 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    5)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    9)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    5)       0.78 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    9)       0.22 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
               O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
               O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
               K
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8 Note
               K
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          9 Note
               K
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          6 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          6 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
                 1  0  0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         70 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.0 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      1.658 Note
               Predicted wR2: Based on SigI**2 10.12 or SHELX Weight 16.26
PLAT984_ALERT_1_G The  K-f'=    0.2030 Deviates from the B&C-Value     0.1927 Check
PLAT984_ALERT_1_G The Mo-f'=   -1.8880 Deviates from the B&C-Value    -1.8622 Check
PLAT985_ALERT_1_G The  K-f"=    0.2500 Deviates from the B&C-Value     0.2361 Check
PLAT985_ALERT_1_G The Mo-f"=    0.6650 Deviates from the B&C-Value     0.6534 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   5 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  27 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  14 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 19/12/2024; check.def file version of 19/12/2024

Datablock 7_cr2_a405nm_a - ellipsoid plot