checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 10_cr3_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: 10_cr3_a405nm_a

Bond precision: N- C = 0.0160 A Wavelength=0.68890

Cell: a=9.598(4) b=9.710(2) c=9.752(3)
alpha=66.10(2) beta=87.91(3) gamma=88.84(3)
Temperature: 30 K

	Calculated	Reported
Volume	830.4(5)	830.4(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C6 Mo N6, C N, 2(O), 4(K)	C7 K3.806 Mo N7 O2, 0.194(K)
Sum formula	C7 K4 Mo N7 O2	C7 K4 Mo N7 O2
Mr	466.48	466.48
Dx,g cm-3	1.866	1.866
Z	2	2
Mu (mm-1)	1.637	1.627
F000	450.0	450.0
F000'	447.80	
h,k,lmax	11,12,12	11,12,12
Nref	3390	3306
Tmin,Tmax	0.943,0.984	0.997,1.000
Tmin'	0.937	

Correction method= # Reported T Limits: Tmin=0.997 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.975 Theta(max)= 25.496

R(reflections)= 0.0567(2293) wR2(reflections)= 0.1444(3306)

S = 0.996 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 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.

Alert level C

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 K3.806 Mo N7 O2, 0.194(K)
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.1 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 72 Report

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

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.93Ang From Mo1B 1.68 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.05Ang From O2B . 0.83 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.05Ang From O1B . 0.77 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.04Ang From O2B . 0.63 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.40Ang From O1B . -0.45 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
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 2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0010 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0010 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note

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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)      0.81 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    9)      0.19 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          2 Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         12 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.9 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      1.213 Note
             Predicted wR2: Based on SigI**2 11.91 or SHELX Weight 14.50
PLAT984_ALERT_1_G The  K-f'=    0.2029 Deviates from the B&C-Value     0.1927 Check
PLAT984_ALERT_1_G The Mo-f'=   -1.8879 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"=    0.6654 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
   2 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  23 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
  12 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 10_cr3_a405nm_a - ellipsoid plot