checkCIF/PLATON report

Structure factors have been supplied for datablock(s) KcryptMoCN6_100K

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: KcryptMoCN6_100K

Bond precision: C-C = 0.0050 A Wavelength=0.71073

Cell: a=18.2778(5) b=20.0943(6) c=43.6202(11)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	16020.8(8)	16020.8(8)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	3(C18 H36 K N2 O6), C6 Mo N6, 2(C2 H3 N)	?
Sum formula	C64 H114 K3 Mo N14 O18	C64 H114 K3 Mo N14 O18
Mr	1580.93	1580.93
Dx,g cm-3	1.311	1.311
Z	8	8
Mu (mm-1)	0.390	0.390
F000	6712.0	6712.0
F000'	6705.75	
h,k,lmax	24,26,57	24,26,57
Nref	19115	19084
Tmin,Tmax	0.869,0.940	0.655,0.746
Tmin'	0.856	

Correction method= # Reported T Limits: Tmin=0.655 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.879

R(reflections)= 0.0667(16415) wR2(reflections)= 0.1242(19084)

S = 1.204 Npar= 903

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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PLAT230_ALERT_2_C Hirshfeld Test Diff for    N11      --C55      .        6.5 s.u.
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C62 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
             C18 H36 K N2 O6
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     12.409 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.462 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          9 Note
               0  2  0,   1  1  1,   0  2  1,   0  0  2,   1  0  2,   1  1  2,
               1  1  3,   0  0  4,   1  0  4,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          6 Report
               2  1  0,   2  1  1,   1  2  1,   1  2  2,   0  2  3,   1  1  4,
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.25Ang From O15            -2.15 eA-3
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Alert level G

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PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      45.11 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo1      --C2       .        7.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo1      --C3       .        6.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo1      --C4       .        8.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo1      --C5       .        5.7 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          3 Note
             H7AB    H8AB    H9AB
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated   and Succeeded by SHELXL     2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         16 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          3 Note
               1  1  4,   1  2  2,   1  0  4,
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..........       3.850 Note
             Predicted wR2: Based on SigI**2  3.23 or SHELX Weight 10.31
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
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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
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   5 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 KcryptMoCN6_100K - ellipsoid plot