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: neu

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Bond precision:  C-C = 0.0080 A          Wavelength=0.71073

Cell:           a=21.2962(11)    b=15.8321(9)      c=32.0204(19)
                alpha=90         beta=94.831(7)    gamma=90
Temperature:    170 K
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	Calculated	Reported
Volume	10757.8(11)	10757.8(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(Mo7 O24), 11(C4 H12 N), C3 H9 N, 8(H2 O), C H3	?
Sum formula	C48 H160 Mo14 N12 O56	C24 H80 Mo7 N6 O28
Mr	3145.04	1572.52
Dx,g cm-3	1.942	1.942
Z	4	8
Mu (mm-1)	1.662	1.662
F000	6272.0	6272.0
F000’	6178.14	
h,k,lmax	25,18,38	25,18,37
Nref	18895	18450
Tmin,Tmax	0.853,0.905	0.736,0.873
Tmin’	0.819	

```
Correction method= # Reported T Limits: Tmin=0.736 Tmax=0.873
AbsCorr = NUMERICAL

Data completeness= 0.976          Theta(max)= 24.966

R(reflections)= 0.0338( 15276)    wR2(reflections)= 0.0893( 18450)

S = 1.020                 Npar= 1201
```

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

PLAT417_ALERT_2_B Short Inter D-H..H-D H9N .. H14O .. 2.04 Ang.
PLAT417_ALERT_2_B Short Inter D-H..H-D H9O .. H12O .. 2.01 Ang.
PLAT417_ALERT_2_B Short Inter D-H..H-D H10O .. H12O .. 2.06 Ang.
PLAT420_ALERT_2_B D-H Without Acceptor O68 -- H16O ... Please Check

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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 numerical
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full ! Check
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 3 Check
PLAT221_ALERT_2_C Solv./Anion Resd 4 C Ueq(max)/Ueq(min) Range 6.0 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 3 H Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 4 H Ueq(max)/Ueq(min) Range 9.6 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 5 H Ueq(max)/Ueq(min) Range 5.1 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 6 H Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd14 H Ueq(max)/Ueq(min) Range 4.8 Ratio
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C111 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C73 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C64 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C72 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H33A .. H84B .. 2.05 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H43A .. H20G .. 2.14 Ang.
PLAT417_ALERT_2_C Short Inter D-H..H-D H5O .. H10O .. 2.11 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1A .. O16 .. 2.61 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H22A .. O23 .. 2.64 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H82A .. O9 .. 2.62 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H92D .. O4 .. 2.62 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H10D .. O32 .. 2.62 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H10E .. O33 .. 2.62 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 25 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 52 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.90 Why ?
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 5 Report
PLAT300_ALERT_4_G Atom Site Occupancy of >C102 is Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C103 is Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C104 is Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C202 is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C203 is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C204 is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10A is Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10B is Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10E is Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10F is Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10G is Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10H is Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10I is Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10J is Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10K is Constrained at 0.6 Check

PLAT300_ALERT_4_G Atom Site Occupancy of <H10C is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H10D is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H20A is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H20B is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H20C is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H20D is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H20E is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H20F is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H20G is Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C62   is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C63   is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C62′ is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C63′ is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H61A is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H61B is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H62A is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H62B is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H63A is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H63B is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H64A is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H64B is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H64C is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H61C is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H61D is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H62C is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H62D is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H63C is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H63D is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H64D is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H64E is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H64F is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C83   is Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C84   is Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C83′ is Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C84′ is Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H82A is Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H82B is Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H83A is Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H83B is Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H84A is Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H84B is Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H84C is Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H82C is Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H82D is Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H83C is Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H83D is Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H84D is Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H84E is Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H84F is Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C92   is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C93   is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C92′ is Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C93′ is Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H91A is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H91B is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H92A is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H92B is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H93A is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H93B is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H94A is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H94B is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H94C is Constrained at 0.65 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of <H91C   is Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H91D   is Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H92C   is Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H92D   is Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H93C   is Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H93D   is Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H94D   is Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H94E   is Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H94F   is Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C112   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C113   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C212   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C213   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H11C   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H11D   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H11E   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H11F   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H11G   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H11H   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H11I   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H11J   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21C   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21D   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21E   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21F   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C114   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H11K   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H11L   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H11M   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C214   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21G   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21H   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21I   is Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =         18 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C93'   --  C94     .      1.85 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C113   --  C114    .      1.79 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C213   --  C214    .      1.76 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
             C4 H12 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8 Note
             C4 H12 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         12 Note
             C4 H12 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         18 Note
             H2 O
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        11 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  22 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 124 ALERT level G = General information/check it is not something unexpected

   3 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
   2 ALERT type 3 Indicator that the structure quality may be low
 131 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 06/05/2016; check.def file version of 05/05/2016

Datablock neu - ellipsoid plot