checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Comp2

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: Comp2

Bond precision: C-C = 0.0171 A Wavelength=0.71073

Cell: a=51.185(12) b=14.237(3) c=24.066(5)
alpha=90 beta=113.204(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	16119(6)	16119(6)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	2(Mo12 O40 P), 3(C24 H22 Fe N10 O2), 2(C H3 N O2) [+ solvent]	2(Mo12 O40 P), 3(C24 H22 Fe N10 O2), 2(C H3 N O2)
Sum formula	C74 H72 Fe3 Mo24 N32 O90 P2 [+ solvent]	C74 H84 Fe3 Mo24 N32 O96 P2
Mr	5381.69	5489.78
Dx,g cm-3	2.218	2.262
Z	4	4
Mu (mm-1)	2.177	2.182
F000	10304.0	10544.0
F000'	10147.79	
h,k,lmax	66,18,31	66,18,31
Nref	18526	18288
Tmin,Tmax	0.770,0.804	0.496,0.746
Tmin'	0.646	

Correction method= # Reported T Limits: Tmin=0.496 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 0.987 Theta(max)= 27.495

R(reflections)= 0.0782(12038) wR2(reflections)= 0.2035(18288)

S = 1.047 Npar= 1018

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

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PLAT420_ALERT_2_B D-H Without Acceptor       O1     --  H34    ...     Please Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O25    ..  N2      ..       2.84 Ang.
PLAT990_ALERT_1_B Deprecated RES file style based SQUEEZE job ....          ! Note
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Alert level C

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CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
           calculated from the _atom_site* data lies outside
           the range 0.99 <> 1.01
          From the CIF: _cell_formula_units_Z                   4
          From the CIF: _chemical_formula_weight          5489.78
          TEST: Calculate formula weight from _atom_site_*
          atom     mass    num     sum
          C        12.01   74.00  888.81
          H         1.01   72.00   72.58
          N        14.01   32.00  448.22
          O        16.00   90.00 1439.91
          P        30.97    2.00   61.95
          Fe       55.85    3.00  167.54
          Mo       95.94   24.00 2302.56
          Calculated formula weight            5381.57
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           yelllow
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT213_ALERT_2_C Atom O5             has ADP max/min Ratio .....        3.7 prolat
PLAT213_ALERT_2_C Atom O16            has ADP max/min Ratio .....        3.2 oblate
PLAT214_ALERT_2_C Atom O1      (Anion/Solvent) ADP max/min Ratio         4.2 prolat
PLAT221_ALERT_2_C Solv./Anion Resd 2   C   Ueq(max)/Ueq(min) Range       4.2 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 2   H   Ueq(max)/Ueq(min) Range       7.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N1     --  C5      ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N4     --  N5      ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C10    --  C11     ..       0.21 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        N16 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2 Note
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01715 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     12.505 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.797 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         40 Report
PLAT977_ALERT_2_C Check the Negative Difference Density on      H8      -0.48 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on     H12      -0.58 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on     H18      -0.50 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on     H19      -0.49 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on     H21      -0.37 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on     H24      -0.89 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on     H26      -0.38 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on     H28      -0.46 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on     H29      -0.33 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on     H30      -0.58 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on     H32      -0.49 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on     H34      -0.78 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Note
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C74 H84 Fe3 Mo24 N32 O96 P2
           Atom count from _chemical_formula_moiety:C74 H72 Fe3 Mo24 N32 O90 P2
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C74 H84 Fe3 Mo24 N32 O96 P2
           Atom count from the _atom_site data:  C74 H72 Fe3 Mo24 N32 O90 P2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C74 H84 Fe3 Mo24 N32 O96 P2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        296.00    296.00    0.00
          H        336.00    288.00   48.00
          Fe        12.00     12.00    0.00
          Mo        96.00     96.00    0.00
          N        128.00    128.00    0.00
          O        384.00    360.00   24.00
          P          8.00      8.00    0.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         40 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum found in CIF ........     Please Check
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group     C2/c       I2/a Note
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          3 Report
PLAT432_ALERT_2_G Short Inter X...Y Contact  O7     ..  C36     ..       2.97 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O8     ..  C13     ..       3.02 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O25    ..  C1      ..       3.01 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O29    ..  C16     ..       3.00 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O30    ..  C25     ..       2.81 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        558 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)           1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        197 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
32 **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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
30 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
11 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock Comp2 - ellipsoid plot