checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Comp1

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: Comp1

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Bond precision:  C-C = 0.0256 A          Wavelength=0.71073

Cell:           a=23.373(12)    b=14.211(8)          c=24.002(14)
                alpha=90        beta=107.455(11)     gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          7605(7)                   7605(8)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
                Mo12 O40 P, C24 H22 Fe N10 Mo12 O40 P, C24 H22 Fe N10
Moiety formula  O2, C16 H36 N, 2(C H3 N   O2, C12 H27 N, 2(C H3 N
                O2)                       O2), C4 H9
Sum formula     C42 H64 Fe Mo12 N13 O46 P C42 H64 Fe Mo12 N13 O46 P
Mr              2725.16                   2725.16
Dx,g cm-3       2.380                     2.380
Z               4                         4
Mu (mm-1)       2.218                     2.218
F000            5280.0                    5280.0
F000'           5201.28
h,k,lmax        30,18,31                  30,18,31
Nref            17476                     17027
Tmin,Tmax       0.766,0.978               0.372,0.746
Tmin'           0.514

Correction method= # Reported T Limits: Tmin=0.372 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 0.974          Theta(max)= 27.494

R(reflections)= 0.0774( 10587)    wR2(reflections)= 0.2019( 17027)

S = 1.058                 Npar= 1045
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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

PLAT031_ALERT_4_B Refined Extinction Parameter within Range ..... 2.333 Sigma
PLAT234_ALERT_4_B Large Hirshfeld Difference N11 -- C33 .. 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference N11 -- C37 .. 0.30 Ang.
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02557 Ang.
PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C39 - C40 .. 1.32 Ang.
PLAT420_ALERT_2_B D-H Without Acceptor O1 -- H63 ... Please Check

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Alert level C

PLAT213_ALERT_2_C Atom O26 has ADP max/min Ratio ..... 3.1 prolat
PLAT223_ALERT_4_C Solv./Anion Resd 3 H Ueq(max)/Ueq(min) Range 5.0 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C33 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C37 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N11 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C38 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C39 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of N12 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.3 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.3 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.8 Note
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C27 - C28 .. 1.34 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C29 - C30 .. 1.43 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C33 - C34 .. 1.39 Ang.
PLAT430_ALERT_2_C Short Inter D...A Contact O16 .. O45 .. 2.88 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 3.166 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 114 Report
PLAT971_ALERT_2_C Check Calcd Residual Density 1.01A From Mo5 1.88 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.89A From C40 1.83 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.28A From C37 1.80 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.96A From Mo8 1.75 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.12A From O23 1.66 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.26A From Mo3 1.65 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.28A From C35 1.64 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.93A From C22 1.64 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.87A From C24 1.63 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.05A From Mo10 1.59 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.87A From O22 1.56 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.07A From C25 1.54 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.06A From Mo1 1.52 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.22A From Mo12 1.52 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.95A From Mo2 1.51 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.92A From Mo10 -2.10 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.83A From Mo1 -2.06 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.74A From Mo4 -1.83 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.79A From Mo3 -1.65 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.78A From Mo8 -1.58 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.72A From Mo7 -1.55 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.93A From Mo12 -1.54 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.97A From Mo6 -1.53 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.78A From Mo5 -1.52 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.70A From Mo2 -1.51 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density 0.69A From O46 -1.21 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H11 -0.41 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H20 -0.52 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H25 -0.70 eA-3

PLAT977_ALERT_2_C Check the Negative Difference Density on H37 -0.36 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H39 -0.33 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H40 -0.86 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H41 -0.47 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H56 -0.33 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H59 -0.31 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H63 -0.35 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Note

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Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 55 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 103.57 Why ?
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 7 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 7 Report
PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C35 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O6 .. C21 .. 2.99 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O8 .. C17 .. 2.86 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O26 .. C4 .. 2.96 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 687 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 335 Note
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ... 61 Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
6 **ALERT level B** = A potentially serious problem, consider carefully
54 **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
58 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
8 ALERT type 4 Improvement, methodology, query or suggestion
1 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 Comp1 - ellipsoid plot