checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ne

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: ne

Bond precision: C-C = 0.0127 A Wavelength=1.54178

Cell: a=22.8582(3) b=23.0300(4) c=23.0373(3)
alpha=90 beta=90.840(1) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	12126.1(3)	12126.1(3)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C16 H34 N, 5(C16 H36 N), 2(C7 N7 Os), O	3(C16 H36 N), (C7 N7 Os), 0.5(H2 O)
Sum formula	C110 H214 N20 O Os2	C55 H109 N10 O0.50 Os
Mr	2213.47	1108.72
Dx,g cm-3	1.212	1.215
Z	4	8
Mu (mm-1)	4.281	4.282
F000	4696.0	4712.0
F000’	4665.92	
h,k,lmax	28,28,28	28,27,28
Nref	24136	23015
Tmin,Tmax	0.720,0.903	0.900,1.000
Tmin’	0.603	

Correction method= # Reported T Limits: Tmin=0.900 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.954 Theta(max)= 72.700

R(reflections)= 0.0541(14167) wR2(reflections)= 0.1418(23015)

S = 0.932 Npar= 1234

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 A

PLAT971_ALERT_2_A Check Calcd Residual Density 1.13A From Os2 4.74 eA-3

Author Response: The crystal was slightly twinned. The residual electron density has no physical meaning for this reason

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Alert level B

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1W Check

Author Response: The atom belongs to solvated water molecule. Due to obvious uncertanty in localization of H atoms in the absence of pronounsed H bonds, H atoms could not be refined in calculated positions.

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 4 Check

Author Response: The crystal was slightly twinned. The residual electron density has no physical meaning for this reason

PLAT971_ALERT_2_B Check Calcd Residual Density 1.04A From Os1 2.96 eA-3

Author Response: The crystal was slightly twinned. The residual electron density has no physical meaning for this reason

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Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.97 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.90 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 1 Check
PLAT220_ALERT_2_C Non-Solvent Resd 6 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C123 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01274 Ang.
PLAT430_ALERT_2_C Short Inter D...A Contact O1W .. N12 .. 2.89 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 4.923 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 321 Report
PLAT971_ALERT_2_C Check Calcd Residual Density 1.04A From Os1 2.06 eA-3

Author Response: The crystal was slightly twinned. The residual electron density has no physical meaning for this reason

PLAT971_ALERT_2_C Check Calcd Residual Density 1.36A From Os2 1.73 eA-3

Author Response: The crystal was slightly twinned. The residual electron density has no physical meaning for this reason

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PLAT971_ALERT_2_C Check Calcd Residual Density  1.15A From     C16       1.66 eA-3
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Author Response: The crystal was slightly twinned. The residual electron density has no physical meaning for this reason

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PLAT972_ALERT_2_C Check Calcd Residual Density  0.90A From     Os1      -1.79 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density  0.68A From     O1W      -0.68 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density  0.60A From     O1W      -0.66 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density  0.73A From     O1W      -0.62 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density  0.60A From     O1W      -0.62 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density  0.81A From     O1W      -0.52 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_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:C55 H109 N10 O0.5 Os1
           Atom count from the _atom_site data:  C55 H107 N10 O0.5 Os1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    8
          From the CIF: _chemical_formula_sum  C55 H109 N10 O0.50 Os
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        440.00    440.00    0.00
          H        872.00    856.00   16.00
          N         80.00     80.00    0.00
          O          4.00      4.00    0.00
          Os         8.00      8.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          7 Note
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for    N25    --  C25     ..        5.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Os1    --  C16     ..        6.3 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of <C64A   is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C64B   is Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C64C   is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C65A   is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C65B   is Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C65C   is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H64C   is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H64D   is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H64E   is Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H64F   is Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H64G   is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H64H   is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H65A   is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H65B   is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H65C   is Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H65D   is Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H65E   is Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H65F   is Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H65G   is Constrained at       0.25 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of <H65H   is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H65I   is Constrained at       0.25 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =          2 Note
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C641   -   C642   ..       1.52 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        652 Check
              C64B -C642 -C64C    1.555   1.555   1.555            38.10 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
              C16 H36 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
              C16 H36 N
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....          15 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL      2014 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        748 Note
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  1 ALERT level A = Most likely a serious problem - resolve or explain
  3 ALERT level B = A potentially serious problem, consider carefully
 21 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 39 ALERT level G = General information/check it is not something unexpected

  7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 22 ALERT type 2 Indicator that the structure model may be wrong or deficient
  8 ALERT type 3 Indicator that the structure quality may be low
 26 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 11/08/2016; check.def file version of 04/08/2016

Datablock ne - ellipsoid plot