checkCIF/PLATON report

Structure factors have been supplied for datablock(s) structure4

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: structure4

Bond precision: C-C = 0.0068 A Wavelength=0.71073

Cell: a=18.2573(4) b=16.2919(5) c=20.8348(5)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	6197.2(3)	6197.2(3)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	4(C40 H80 O16 Ti4), C14 H16	Ti4 O16 C40 H80, 0.5(C7 H8)
Sum formula	C174 H336 O64 Ti16	C43.50 H84 O16 Ti4
Mr	4218.35	1054.70
Dx,g cm-3	1.130	1.130
Z	1	4
Mu (mm-1)	0.549	0.549
F000	2244.0	2244.0
F000’	2249.47	
h,k,lmax	22,20,26	22,20,26
Nref	6577	6567
Tmin,Tmax	0.789,0.864	0.747,0.867
Tmin’	0.734	

Correction method= NUMERICAL

Data completeness= 0.998 Theta(max)= 26.370

R(reflections)= 0.0532(4506) wR2(reflections)= 0.1903(6567)

S = 1.034 Npar= Npar = 425

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

PLAT213_ALERT_2_A Atom C66 has ADP max/min Ratio ..... 6.7 prolat

Author Response: Atom C66 already occurs with partial occupancy and further position splitting is not justified by the data quality.

PLAT234_ALERT_4_A Large Hirshfeld Difference C15 -- C17 .. 0.32 Ang.

Author Response: C15 atom is fully occupied and is the last stable atom in the 2,2'-dim moiety. C17 atom belong to disordered groups rotating along C14-C15 bond.

Alert level B

Crystal system given = orthorhombic
PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C15 Check
PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C25 Check
PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C42 Check
PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C52 Check
PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C62 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 3 Check

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Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.31 Why ?
PLAT213_ALERT_2_C Atom C64 has ADP max/min Ratio ..... 3.2 prolat

Author Response: Atom C66 already occurs with partial occupancy and further position splitting is not justified by the data quality.

PLAT215_ALERT_3_C Disordered C16 has ADP max/min Ratio 3.4
PLAT215_ALERT_3_C Disordered C44 has ADP max/min Ratio 3.5
PLAT215_ALERT_3_C Disordered C65 has ADP max/min Ratio 3.3
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 4.8 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for O21 -- C23 .. 6.5 su
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0068 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H18B .. H86B .. 1.88 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -2.443 Why ?
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 4 Why ?
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 3 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much smaller I(calc) . 1 Check

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Alert level G

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:C43.5 H84 O16 Ti4
Atom count from the _atom_site data: C43.5 H83.5 O16 Ti4
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?

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           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  C43.50 H84 O16 Ti4
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        174.00    174.00    0.00
           H        336.00    334.00    2.00
           O         64.00     64.00    0.00
           Ti        16.00     16.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        15 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by .............      0.25 Ratio
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.12 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ............. Percentage =       29 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         2 Note
            C14 H16
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       12 Note
PLAT910_ALERT_3_G Missing # of FCF Reflections Below Th(Min) .....        4 Why ?
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        2 Note
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  13 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 ALERT type 2 Indicator that the structure model may be wrong or deficient
  12 ALERT type 3 Indicator that the structure quality may be low
   3 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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock structure4 - ellipsoid plot