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: 56_11_1

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Bond precision:  O- O = 0.0400 A         Wavelength=0.71075

Cell:            a=23.525(5)     b=32.926(7)         c=25.424(6)
                 alpha=90        beta=93.273(2)      gamma=90
Temperature:     150 K
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	Calculated	Reported
Volume	19661(8)	19661(7)
Space group	P 21/a	P 21/a
Hall group	-P 2yab	?
Moiety formula	2(In10 O157 Si4 W36), O4, 68(O), 23(K)	?
Sum formula	In20 K23 O386 Si8 W72	In10 K11.50 O193 Si4 W36
Mr	22832.88	11416.81
Dx,g cm-3	3.857	3.857
Z	2	4
Mu (mm-1)	22.491	22.491
F000	19890.0	19890.0
F000’	19778.10	
h,k,lmax	30,42,33	30,42,33
Nref	45058	44125
Tmin,Tmax	0.216,0.325	0.660,1.000
Tmin’	0.008	

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Correction method= # Reported T Limits: Tmin=0.660 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.979          Theta(max)= 27.480

R(reflections)= 0.0829( 34297)    wR2(reflections)= 0.2295( 44125)

S = 1.056                 Npar= 2113
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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 A

PLAT213_ALERT_2_A Atom O47 has ADP max/min Ratio ..... 8.7 prolat
PLAT213_ALERT_2_A Atom O48 has ADP max/min Ratio ..... 5.6 prolat
PLAT213_ALERT_2_A Atom O54 has ADP max/min Ratio ..... 6.6 prolat
PLAT213_ALERT_2_A Atom O55 has ADP max/min Ratio ..... 7.9 prolat
PLAT213_ALERT_2_A Atom O58 has ADP max/min Ratio ..... 10.4 prolat
PLAT213_ALERT_2_A Atom O139 has ADP max/min Ratio ..... 11.5 prolat
PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

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Alert level B

DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00
_refine_diff_density_min given = -8.740
Test value = -7.400
DIFMX01_ALERT_2_B The maximum difference density is > 0.1*ZMAX*1.00
_refine_diff_density_max given = 11.090
Test value = 7.400
PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 11.09 eA-3
PLAT098_ALERT_2_B Large Reported Min. (Negative) Residual Density -8.74 eA-3
PLAT213_ALERT_2_B Atom O10 has ADP max/min Ratio ..... 4.6 prolat
PLAT213_ALERT_2_B Atom O41 has ADP max/min Ratio ..... 4.7 prolat
PLAT213_ALERT_2_B Atom O52 has ADP max/min Ratio ..... 4.1 prolat
PLAT213_ALERT_2_B Atom O53 has ADP max/min Ratio ..... 4.2 prolat
PLAT213_ALERT_2_B Atom O154 has ADP max/min Ratio ..... 4.1 prolat
PLAT220_ALERT_2_B Large Non-Solvent O Ueq(max)/Ueq(min) Range 9.7 Ratio
PLAT234_ALERT_4_B Large Hirshfeld Difference W16 -- O47 .. 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference W18 -- O55 .. 0.26 Ang.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O55 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O158 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O159 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O160 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O161 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O162 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O163 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O164 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O165 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O167 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O168 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O169 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O170 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O171 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O172 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O173 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O174 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O175 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O176 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O178 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O179 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O180 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O181 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O182 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O183 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O184 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O185 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O186 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O187 Check

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PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O188 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O189 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O190 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O191 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O192 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O193 Check
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Alert level C

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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 Multi-scan
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........        36 Check
PLAT213_ALERT_2_C Atom W16             has ADP max/min Ratio .....       3.8 prolat
PLAT213_ALERT_2_C Atom W17             has ADP max/min Ratio .....       3.8 prolat
PLAT213_ALERT_2_C Atom W18             has ADP max/min Ratio .....       3.6 prolat
PLAT213_ALERT_2_C Atom O15             has ADP max/min Ratio .....       3.1 prolat
PLAT213_ALERT_2_C Atom O36             has ADP max/min Ratio .....       3.5 prolat
PLAT213_ALERT_2_C Atom O45             has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom O49             has ADP max/min Ratio .....       3.5 prolat
PLAT213_ALERT_2_C Atom O56             has ADP max/min Ratio .....       3.6 prolat
PLAT213_ALERT_2_C Atom O57             has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom O66             has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom O90             has ADP max/min Ratio .....       3.6 oblate
PLAT213_ALERT_2_C Atom O127            has ADP max/min Ratio .....       3.5 oblate
PLAT220_ALERT_2_C Large Non-Solvent  W     Ueq(max)/Ueq(min) Range       4.8 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference W10    --  O46     ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference W15    --  O45     ..      0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference W15    --  O46     ..      0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference In10   --  O157    ..      0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O41 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O47 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O52 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O66 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.2 Note
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         1 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF     Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ............      0.50 Ratio
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large   1091.54 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  P21/a     P21/c   Note
PLAT793_ALERT_4_G The Model has Chirality at Si1     (Centro SPGR)         R Verify
PLAT793_ALERT_4_G The Model has Chirality at Si2     (Centro SPGR)         S Verify
PLAT793_ALERT_4_G The Model has Chirality at Si3     (Centro SPGR)         R Verify
PLAT793_ALERT_4_G The Model has Chirality at Si4     (Centro SPGR)         R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for In5     (III)   .....      3.02 Note
PLAT794_ALERT_5_G Tentative Bond Valency for In6     (III)   .....      3.03 Note
PLAT794_ALERT_5_G Tentative Bond Valency for In7     (III)   .....      2.80 Note
PLAT794_ALERT_5_G Tentative Bond Valency for In8     (III)   .....      2.94 Note
PLAT794_ALERT_5_G Tentative Bond Valency for In9     (III)   .....      2.92 Note
PLAT794_ALERT_5_G Tentative Bond Valency for In10    (III)   .....      2.96 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         6 Note
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PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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  7 ALERT level A = Most likely a serious problem - resolve or explain
 47 ALERT level B = A potentially serious problem, consider carefully
 26 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 19 ALERT level G = General information/check it is not something unexpected

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 73 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
 12 ALERT type 4 Improvement, methodology, query or suggestion
  8 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 19/11/2015; check.def file version of 17/11/2015

Datablock 56_11_1 - ellipsoid plot