checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4

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: 4

Bond precision: C-C = 0.0104 A Wavelength=1.54184

Cell: a=12.8836(4) b=17.0564(6) c=18.6427(5)
alpha=108.840(3) beta=90.263(2) gamma=91.142(3)
Temperature: 100 K

	Calculated	Reported
Volume	3876.2(2)	3876.2(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H72 Cl Si8 Th, C24 H48 Cl3 Mg2 O6	C32 H72 Cl Si8 Th, C24 H48 Cl3 Mg2 O6
Sum formula	C56 H120 Cl4 Mg2 O6 Si8 Th	C56 H120 Cl4 Mg2 O6 Si8 Th
Mr	1536.70	1536.69
Dx,g cm-3	1.317	1.317
Z	2	2
Mu (mm-1)	9.126	9.126
F000	1596.0	1596.0
F000'	1598.18	
h,k,lmax	15,20,22	15,20,22
Nref	14211	14120
Tmin,Tmax	0.309,0.694	0.411,0.770
Tmin'	0.202	

Correction method= # Reported T Limits: Tmin=0.411 Tmax=0.770
AbsCorr = ANALYTICAL

Data completeness= 0.994 Theta(max)= 68.251

R(reflections)= 0.0415(12331) wR2(reflections)= 0.1093(14120)

S = 1.026 Npar= 1161

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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.51Ang From Th1 3.13 eA-3

Author Response: The residual electron density has no chemical meaning and is the result of absorption effects due to a combination of using Cu/Ka, the heavy Th metal centre and the shape of the crystal This is a common occurence with SC-XRD diffraction data collected using Cu/Ka of compounds containing heavy scaterrers such as U and Th We have tried different absorption correction methods and the numerical absorption correction based on crystal faces as described by Clark and Reid has given the best results Absorption correction based on multi-scan gave worse Rint and higher residual density around the Th metal centre Unfortunately due to the size of the crystal our laboratory's Mo/Ka source was inadequate to collect data with the required resolution and intensity for anything else other than providing connectivity

Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.76	Report
PLAT213_ALERT_2_C	Atom C23A has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.9	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference Th1 --C6A .	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Th1 --C7A .	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Si3 --C15 .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Mg2 --O3A .	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C34 --C35A .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C35A --C36A .	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C39 --C40 .	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C40 --C41 .	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C45 --C44A .	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C51 --C52 .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C55 --C54 .	0.16	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C34	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C37	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C48	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01043	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	80	Report
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.60Ang From C34 .	-0.53	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H55A .	-0.34	eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	105	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	29	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.33	Why ?
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	2	Note
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report

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PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        126 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          9 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    Si3      --C16      .        6.4 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O1       --C34      .        7.6 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O1       --C37      .        5.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cl0A     --Mg2      .        7.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cl2      --Mg1      .       14.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cl0B     --Mg1      .       12.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mg2      --O3       .        5.6 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        55% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        66% Note
PLAT303_ALERT_2_G Full Occupancy Atom H3        with # Connections       2.00 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  H48B     ..H40D     .       2.02 Ang.
                                                  -1+x,y,z  =      1_455 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H10B     ..H28D     .       1.99 Ang.
                                                  x,y,z  =         1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H19A     ..H22A     .       2.06 Ang.
                                                  x,y,z  =         1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H19A     ..H24F     .       1.99 Ang.
                                                  x,y,z  =         1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          2 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C34      --C35             1.77 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C38      --C39             1.74 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C38A     --C39A            1.80 Ang.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        576 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
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          8 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
21 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
34 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
29 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
19 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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checkCIF publication errors

Alert level A

```
PUBL004_ALERT_1_A  The contact author's name and address are missing,
           _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
           _publ_contact_author_phone are all missing.
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            At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
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   7 ALERT level A = Data missing that is essential or data in wrong format
   0 ALERT level G = General alerts. Data that may be required is missing
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Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
```

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RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock 4 - ellipsoid plot