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: JK22_3

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Bond precision:  Si- C = 0.0020 A        Wavelength=0.71073

Cell:           a=11.5359(16)    b=6.7079(9)        c=10.1493(13)
                alpha=90         beta=115.830(4)    gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          706.90(17)                706.90(17)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C10 H22 O5 Si2            C10 H22 O5 Si2
Sum formula     C10 H22 O5 Si2            C10 H22 O5 Si2
Mr              278.46                    278.45
Dx,g cm-3       1.308                     1.308
Z               2                         2
Mu (mm-1)       0.258                     0.258
F000            300.0                     300.0
F000'           300.47
h,k,lmax        13,8,12                   13,8,12
Nref            1312                      1303
Tmin,Tmax       0.958,0.985               0.821,1.000
Tmin'           0.950

Correction method= # Reported T Limits: Tmin=0.821 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.993          Theta(max)= 25.500

R(reflections)= 0.0326( 1107)     wR2(reflections)= 0.0873( 1303)

S = 1.095                 Npar= 125
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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 G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 13 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report

Author Response: The positions of the H atoms of the OH groups were taken from a difference Fourier map, the O-H distances were fixed to 0.84A, and the H atoms were refined with common isotropic displacement parameters without any constraints to the bond angles (DFIX of SHELXL).

PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 2 Report

Author Response: The Si and O atoms were refined without any constraints. The cyclopentyl groups are disordered over two orientations and were refined with site occupation factors of 0.5. The equivalent bonds in these groups were restrained to have the same lengths (SAME instruction of SHELXL). The non-hydrogen atoms were refined with anisotropic displacement parameters.

PLAT300_ALERT_4_G Atom Site Occupancy of C21 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C32 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C41 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C42 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C51 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C52 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H211 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H212 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H221 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H222 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H311 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H312 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H321 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H322 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H411 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H412 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H421 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H422 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H511 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H512 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H521 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H522 is Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1).. 47% Note
PLAT396_ALERT_2_G Deviating Si-O-Si Angle from 150 Deg for O1 180.0 Degree
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 28 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 4 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

32 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
26 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: JK22_5B

Bond precision: Si- C = 0.0030 A Wavelength=0.71073

Cell: a=10.1476(5) b=20.7484(10) c=6.7022(3)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1411.13(12)	1411.12(12)
Space group	C m c a	C m c a
Hall group	-C 2bc 2	-C 2bc 2
Moiety formula	C10 H22 O5 Si2	C10 H22 O5 Si2
Sum formula	C10 H22 O5 Si2	C10 H22 O5 Si2
Mr	278.46	278.45
Dx,g cm-3	1.311	1.311
Z	4	4
Mu (mm-1)	0.258	0.258
F000	600.0	600.0
F000’	600.93	
h,k,lmax	12,25,8	12,25,8
Nref	741	734
Tmin,Tmax	0.923,0.970	0.801,1.000
Tmin’	0.907	

Correction method= # Reported T Limits: Tmin=0.801 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 26.000

R(reflections)= 0.0344(683) wR2(reflections)= 0.0903(734)

S = 1.159 Npar= 66

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 G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         3 Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         1 Report
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Author Response: The cyclopentyl group is disordered over two orientations and was refined with site occupation factors of 0.5. The same anisotropic displacement parameters were used for atoms C2 and C5 (EADP instruction of SHELXL). All other non-hydrogen atoms were refined with anisotropic displacement parameters without any constraints.

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PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 Report
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Author Response: The positions of the disordered H atoms of the OH groups were taken from a difference Fourier map, the O-H distances were fixed to 0.84A, and the H atoms were refined with site occupation factors of 0.5 and common isotropic displacement parameters without any constraints to the bond angles (DFIX of SHELXL).

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PLAT300_ALERT_4_G Atom Site Occupancy of C2      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H51     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52     is Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1)..        47% Note
PLAT396_ALERT_2_G Deviating Si-O-Si Angle from 150 Deg for  O1         180.0 Degree
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         3 Note
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   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 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
  16 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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Datablock: JK66_4C

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Bond precision:  C-C = 0.0028 A          Wavelength=0.71073
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Cell:	a=16.2855(8)	b=22.3460(11)	c=19.6563(9)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	7153.2(6)	7153.2(6)
Space group	C c c a	C c c a
Hall group	-C 2b 2bc	-C 2b 2bc
Moiety formula	C30 H54 O9 Si6	C30 H54 O9 Si6
Sum formula	C30 H54 O9 Si6	C30 H54 O9 Si6
Mr	727.27	727.27
Dx,g cm-3	1.351	1.351
Z	8	8
Mu (mm-1)	0.283	0.283
F000	3120.0	3120.0
F000’	3125.11	
h,k,lmax	22,31,27	22,31,27
Nref	5233	5219
Tmin,Tmax	0.897,0.950	0.802,1.000
Tmin’	0.893	

Correction method= # Reported T Limits: Tmin=0.802 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 30.000

R(reflections)= 0.0378(4062) wR2(reflections)= 0.1049(5219)

S = 1.052 Npar= 213

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 C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C33 -- C34 .. 5.5 s.u.
PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C24 Check
PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C34 Check

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Alert level G

PLAT396_ALERT_2_G Deviating Si-O-Si Angle from 150 Deg for O1 128.7 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si Angle from 150 Deg for O2 131.3 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si Angle from 150 Deg for O3 131.1 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si Angle from 150 Deg for O4 139.8 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si Angle from 150 Deg for O5 132.3 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact Si2 .. O1 .. 3.36 Ang.
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note

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  0 ALERT type 4 Improvement, methodology, query or suggestion
  0 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

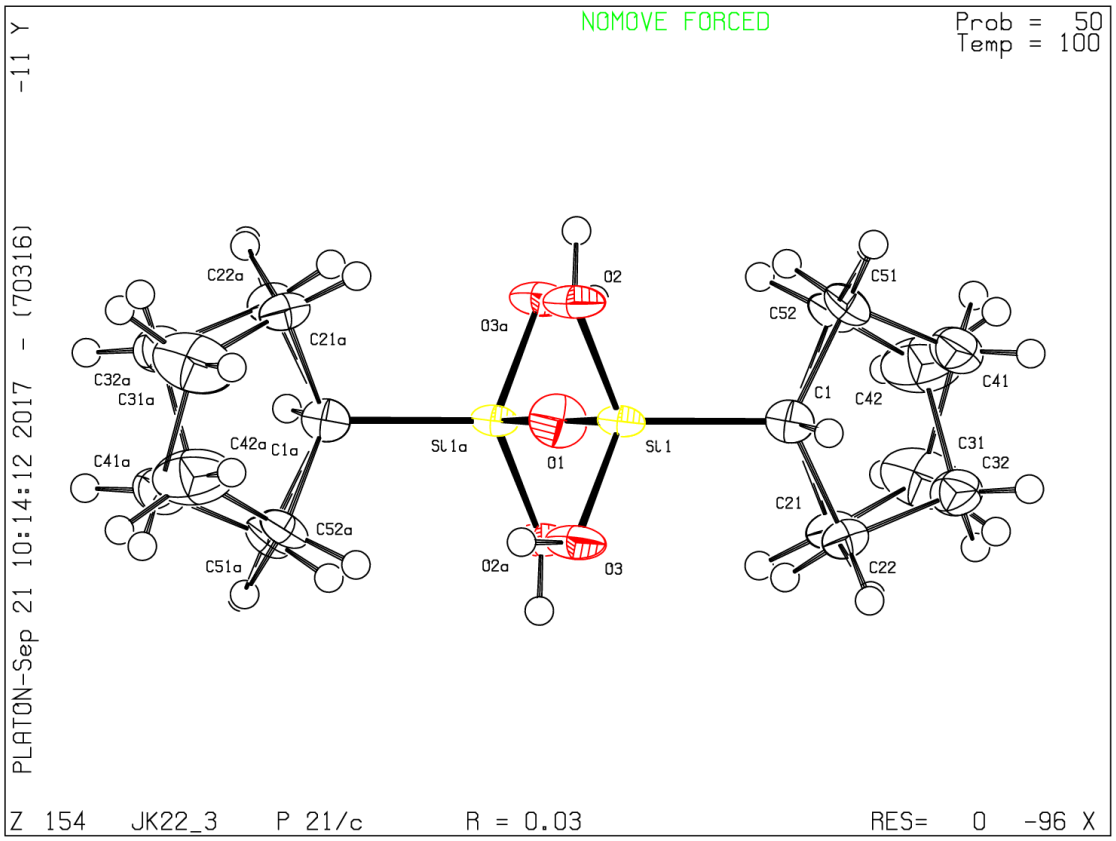
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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

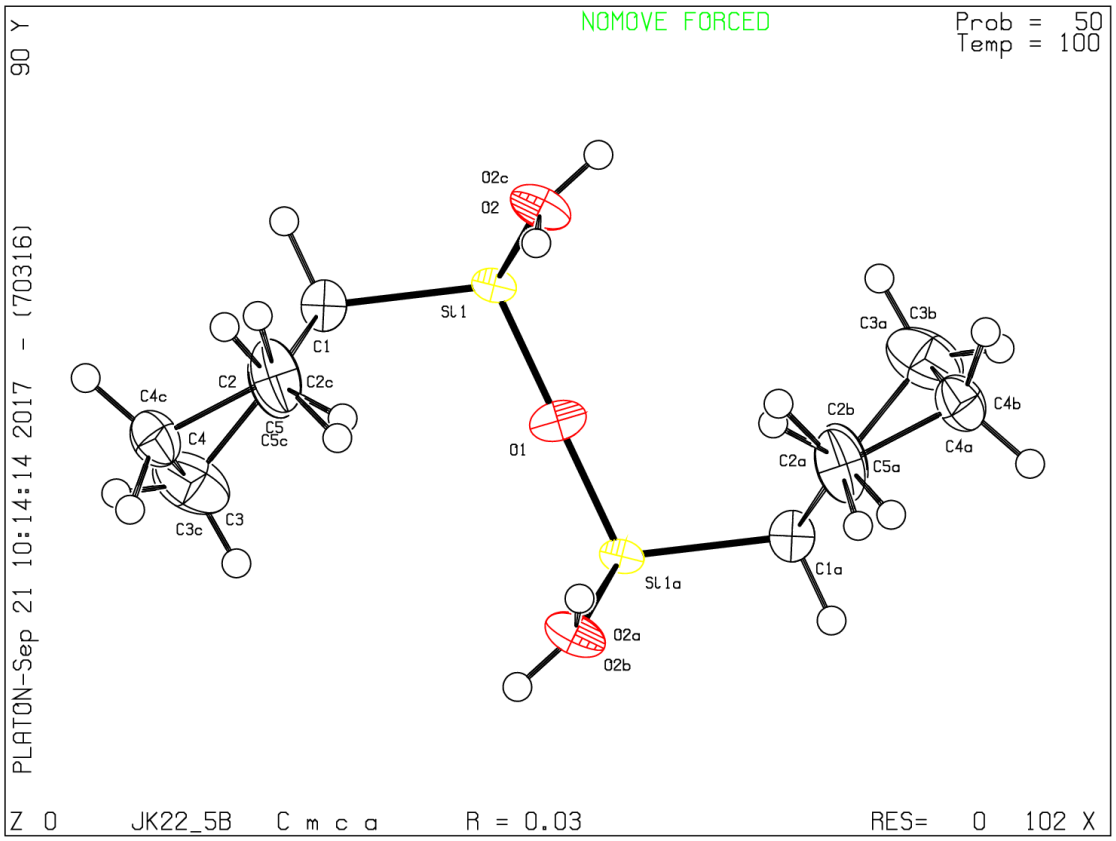
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/08/2017; check.def file version of 27/07/2017

Datablock JK22_3 - ellipsoid plot



Datablock JK22_5B - ellipsoid plot



Datablock JK66_4C - ellipsoid plot