checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tps214orthoacent

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: tps214orthoacent

```
Bond precision:  C-C = 0.0053 A          Wavelength=0.71073

Cell:              a=10.287(2)      b=11.429(2)      c=20.495(4)
                   alpha=90         beta=90          gamma=90
Temperature:       100 K
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	Calculated	Reported
Volume	2409.6(8)	2409.6(8)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C22 H37 K O2 Si	C22 H37 K O2 Si
Sum formula	C22 H37 K O2 Si	C22 H37 K O2 Si
Mr	400.71	400.70
Dx,g cm-3	1.105	1.096
Z	4	4
Mu (mm-1)	0.282	0.282
F000	872.0	872.0
F000’	873.41	
h,k,lmax	12,14,25	12,14,25
Nref	4777[2714]	4731
Tmin,Tmax	0.935,0.971	0.925,0.971
Tmin’	0.911	

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Correction method= # Reported T Limits: Tmin=0.925 Tmax=0.971
AbsCorr = INTEGRATION

Data completeness= 1.74/0.99      Theta(max)= 26.104

R(reflections)= 0.0380( 3955)     wR2(reflections)= 0.0913( 4731)

S = 0.993                 Npar= 260
```

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

```
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 integration
REFLE01_ALERT_3_C  The _reflns_threshold_multiplier given is >= 4
           Premultiplier =    4.00
REFLE01_ALERT_3_C  The _reflns_threshold_multiplier given is >= 4
           Premultiplier =    4.00
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range        4.9 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00529 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          8 Report
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Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19C    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19D    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20C    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20D    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21C    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21D    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22C    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22D    is Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1)..          8 % Note
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for         C6 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for         C7 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for         C8 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for         C9 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for        C10 Check
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C7     -   C11    ..       1.51 Ang.
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C8     -   C12    ..       1.51 Ang.
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C9     -   C13    ..       1.51 Ang.
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C10    -   C14    ..       1.50 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         18 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 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
8 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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 13 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 ALERT type 3 Indicator that the structure quality may be low
 21 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 27/03/2017; check.def file version of 24/03/2017

Datablock tps214orthoacent - ellipsoid plot