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: compound4

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Bond precision:  C-C = 0.0075 A          Wavelength=0.71073

Cell:           a=14.9582(7)    b=12.6454(6)        c=16.3325(8)
                alpha=90        beta=104.950(2)     gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          2984.8(2)                 2984.8(2)
Space group     C c                       C 1 c 1
Hall group      C -2yc                    C -2yc
                C18 H31.34 O6 Si2, F6 P,  C18 H32 O6 Si2, H4 N,
Moiety formula  0.221(C H2 Cl2), 0.78(C H2 1.28(C0.78 H1.56 Cl1.56),
                Cl), 0.779(               F6 P
Sum formula     C19 H38 Cl2 F6 N O6 P Si2 C19 H38 Cl2 F6 N O6 P Si2
Mr              648.59                    648.55
Dx,g cm-3       1.443                     1.443
Z               4                         4
Mu (mm-1)       0.422                     0.422
F000            1352.1                    1352.0
F000'           1355.11
h,k,lmax        18,16,20                  18,16,20
Nref            6370[ 3189]               6355
Tmin,Tmax       0.948,0.968               0.698,0.745
Tmin'           0.802

Correction method= # Reported T Limits: Tmin=0.698 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.99/1.00      Theta(max)= 26.785

R(reflections)= 0.0535( 5664)     wR2(reflections)= 0.1329( 6355)

S = 1.035                 Npar= 461
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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 C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ..... 6.92 Note

Author Response: Dist. & Uij restr. needed to model intrinsic disorder caused by DCM.

PLAT213_ALERT_2_C Atom Si1A has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C2 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C1A has ADP max/min Ratio ..... 3.3 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.0 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 4.5 Ratio
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.0 Note
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0075 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 25 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 22 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.37 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 6 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 2 Report
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P1 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1).. 27% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3).. 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4).. 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5).. 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6).. 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (57.34) in Resd. # 1 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (1.11) in Resd. # 3 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (1.87) in Resd. # 4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (1.25) in Resd. # 5 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.78) in Resd. # 6 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.11) in Resd. # 8 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.11) in Resd. # 9 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.11) in Resd. # 10 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.11) in Resd. # 11 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.11) in Resd. # 12 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.11) in Resd. # 13 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle from 120 Deg for >O6 118.3 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle from 120 Deg for <O6A 123.9 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si Angle from 150 Deg for O1 48.0 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle from 120 Deg for O2 109.5 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 19 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 26 Check
C19 -CL1 -C19A 1.555 1.555 1.555 19.00 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 543 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

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

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 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
 25 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 13/08/2017; check.def file version of 27/07/2017

Datablock compound4 - ellipsoid plot