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: I

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Bond precision:   Si- O = 0.0123 A         Wavelength=0.02508

Cell:                a=7.48650      b=17.84630      c=25.65450
                     alpha=90       beta=90         gamma=90
Temperature:         103 K

                 Calculated                  Reported
Volume           3427.603                    3428
Space group      P m m n                     P m m n
Hall group       -P 2ab 2a                   -P -2xa;-2y
                 Na1.80 O120 Si60,
Moiety formula   0.636(O2), 3.54(O),         ?
                 6.36(Na)
Sum formula      Na8.16 O124.81 Si60         Na8.154744 O124.8117 Si60
Mr               3869.90                     3869.50
Dx,g cm-3        1.875                       1.875
Z                1                           1
Mu (mm-1)        0.000                       0.000
F000             0.0                         635.6
F000'            1927.93
h,k,lmax                                     9,23,31
Nref                                         17481
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness=                 Theta(max)= 1.010

                                                wR2(reflections)=
R(reflections)= 0.0966( 1040)                   0.2245( 17481)
S = 0.798                  Npar= 275
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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

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

Author Response: A table of bond angles are already given in the supplementary files.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.
GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.
SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 5.923
Additional refinement cycles may be required.
PLAT080_ALERT_2_A Maximum Shift/Error ..... 5.92 Why ?

Si1	Si2	Si3	Si4	Si5	Si6	Si7	Si8
Si9	Si10	O1	O2	O3	O4	O5	O6
O7	O8	O9	O10	O11	O12	O13	O14
O15	O16	O17	O18	O19	O20	O21	O22
O23							

Author Response: This is related to 3D ED data and dynamical refinements.

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.184
PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ..... 0.184 Report
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Si4 Check
PLAT601_ALERT_2_B Unit Cell Contains Solvent Accessible VOIDS of . 177 Ang**3

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 0.798
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Na8.16 O124.81 Si60
Rep.: Na8.154744 O124.8117 Si60
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -P -2xa;-2 Check
PLAT141_ALERT_4_C s.u. on a - Axis Small or Missing ..... 0.00000 Ang.
PLAT142_ALERT_4_C s.u. on b - Axis Small or Missing ..... 0.00000 Ang.
PLAT143_ALERT_4_C s.u. on c - Axis Small or Missing ..... 0.00000 Ang.
PLAT151_ALERT_1_C No s.u. (esd) Given on Volume ..... Please Do !
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 4 Check

Ow1	Ow2	Na1	Na2

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O1 Check

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O11 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O14 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O15 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O16 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O18 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O19 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O20 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si7 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si8 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Si10 Check
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         2% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% 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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    7)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    8)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    9)       100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        Ow1 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        Ow2 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        Ow4 Check
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O2       .      137.7 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O4       .      177.0 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O10      .      139.3 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O14      .      132.3 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O15      .      139.0 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O17      .      138.4 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O18      .      160.4 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O23      .      180.0 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          4 Note
               Ow1     Ow2     Ow3     Ow4
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        17 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of        3.0 Sig(I)
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   5 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  28 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  28 ALERT level G = General information/check it is not something unexpected
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  8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 35 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
 14 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 06/01/2024; check.def file version of 05/01/2024

Datablock I - ellipsoid plot