



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: p0

Bond precision:	O- C = 0.0100 Å	Wavelength=0.41122	
Cell:	a=10.378 (2)	b=10.378 (2)	c=6.260 (2)
	alpha=90	beta=90	gamma=120
Temperature:	293 K		
	Calculated	Reported	
Volume	583.9 (3)	583.8 (2)	
Space group	P 63 m c	P 63 m c	
Hall group	P 6c -2c	P 6c; -2c	
Moiety formula	C3 O9, 2 (C O3), 4 (Ca), 2 (Na)	?	
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15	
Mr	506.35	506.30	
Dx, g cm ⁻³	2.880	2.880	
Z	2	2	
Mu (mm ⁻¹)	0.442	0.435	
F000	504.0	504.0	
F000'	504.79		
h, k, lmax	17, 17, 10	16, 14, 5	
Nref	1184 [634]	504	
Tmin, Tmax	0.979, 0.991	0.896, 1.000	
Tmin'	0.974		

Correction method= # Reported T Limits: Tmin=0.896 Tmax=1.000
AbsCorr = MULTII-SCAN

Data completeness= 0.79/0.43

Theta(max)= 20.830

R(reflections)= 0.0326(470)

wR2(reflections)=
0.0912(504)

S = 1.630

Npar= 51

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

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low	11.55 Degree
PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low .	0.660 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	19.10 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	19.10 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	30.16 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang)	03 Check

Alert level G

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	1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..	Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O1	8.62 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for C2	6.35 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O2	7.10 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O3	6.03 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O4	8.04 Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K)	293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G Short Inter X...Y Contact O1 ..C2 .	2.58 Ang.
	x-y,x,1/2+z = 6_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C1 ..C1 .	3.13 Ang.
	x-y,x,-1/2+z = 6_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C1 ..C1 .	3.13 Ang.
	x-y,x,1/2+z = 6_555 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .	5.25 Ratio
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ	3 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ	5 Units

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.660 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1 18.05 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1 18.05 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2 32.09 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) 03 Check

Alert level G

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 1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka 0.41122 Ang.
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O1 9.30 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for C2 6.77 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O2 7.74 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O3 5.11 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O4 8.33 Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca1 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na1 Constrained at 0.6667 Check
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
PLAT432_ALERT_2_G Short Inter X...Y Contact O1 ..C2 . 2.57 Ang.
x-y,x,1/2+z = 6_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O2 ..C3 . 3.00 Ang.
1+x-y,x,1/2+z = 6_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl1 ..C1 . 3.11 Ang.
x-y,x,-1/2+z = 6_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl1 ..C1 . 3.11 Ang.
x-y,x,1/2+z = 6_555 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 5.25 Ratio
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 5 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 2 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ 5 Units

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
25 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
5 ALERT type 5 Informative message, check

Datablock: p2

Bond precision: O- C = 0.0090 A Wavelength=0.41122

Cell: a=10.296(2) b=10.296(2) c=6.188(2)
alpha=90 beta=90 gamma=120

Temperature: 293 K

	Calculated	Reported
Volume	568.1(3)	568.1(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx,g cm-3	2.960	2.960
Z	2	2
Mu (mm-1)	0.454	0.447
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	16,17,6
Nref	1180[632]	527
Tmin,Tmax	0.979,0.991	
Tmin'	0.974	

Correction method= Not given

Data completeness= 0.83/0.45 Theta(max)= 20.990

R(reflections)= 0.0376(483) wR2(reflections)=
0.0952(527)

S = 1.293 Npar= 51

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.660 Why?

 Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for Na1 18.03 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for Ca1 18.03 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for Ca2 28.55 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) 03 Check

 Alert level G

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 1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka 0.41122 Ang.
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O1 9.25 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for C2 6.68 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O2 8.01 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O3 5.71 Check
PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O4 8.59 Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca1 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na1 Constrained at 0.6667 Check
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
PLAT432_ALERT_2_G Short Inter X...Y Contact O1 ..C2 . 2.58 Ang.
x-y,x,1/2+z = 6_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O2 ..C3 . 2.98 Ang.
1+x-y,x,1/2+z = 6_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C1 ..C1 . 3.09 Ang.
x-y,x,-1/2+z = 6_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C1 ..C1 . 3.09 Ang.
x-y,x,1/2+z = 6_555 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 5.75 Ratio
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ 4 Units

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
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23 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 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
-

Datablock: p3

Bond precision: O- C = 0.0070 Å Wavelength=0.41122

Cell: a=10.258(2) b=10.258(2) c=6.146(2)
alpha=90 beta=90 gamma=120

Temperature: 293 K

	Calculated	Reported
Volume	560.1(3)	560.1(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c; -2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm ⁻³	3.002	3.002
Z	2	2
Mu (mm ⁻¹)	0.461	0.454
F000	504.0	504.0
F000'	504.79	
h, k, lmax	17, 17, 10	17, 13, 6
Nref	1176[630]	523
Tmin, Tmax	0.978, 0.991	0.868, 1.000
Tmin'	0.973	

Correction method= # Reported T Limits: Tmin=0.868 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.83/0.44 Theta(max)= 21.080

R(reflections)= 0.0272(494) wR2(reflections)=
0.0674(523)

S = 1.214 Npar= 51

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.670 Why?

Alert level C

PLAT034_ALERT_1_C	No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C	Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C	max(sig)/min(sig) ratio x,y,z > 3 for NA1	19.47 Check
PLAT160_ALERT_4_C	max(sig)/min(sig) ratio x,y,z > 3 for CA1	19.47 Check
PLAT160_ALERT_4_C	max(sig)/min(sig) ratio x,y,z > 3 for CA2	25.96 Check
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)	03 Check



Alert level G

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	1 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	8.39 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	6.91 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	8.17 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.24 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	8.99 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.56 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.97 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.07 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.07 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	5.75 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	4 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	4 Units

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check
-

Datablock: p4

Bond precision: O- C = 0.0090 Å Wavelength=0.41122

Cell: a=10.225(2) b=10.225(2) c=6.123(2)
alpha=90 beta=90 gamma=120

Temperature: 293 K

	Calculated	Reported
Volume	554.4(3)	554.4(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.033	3.033
Z	2	2
Mu (mm-1)	0.466	0.459
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	17,13,6
Nref	1174[629]	525
Tmin,Tmax	0.978,0.991	
Tmin'	0.973	

Correction method= Not given

Data completeness= 0.83/0.45 Theta(max)= 21.150

R(reflections)= 0.0338(491) wR2(reflections)=
0.0852(525)

S = 1.298 Npar= 51

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.680 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	20.36 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	20.36 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	33.93 Check

PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang)

03 Check



Alert level G

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 1 Info

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !

PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check

PLAT092_ALERT_4_G Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka 0.41122 Ang.

PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O1 9.80 Check

PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for C2 7.49 Check

PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O2 8.75 Check

PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O3 5.99 Check

PLAT160_ALERT_4_G max(sig)/min(sig) ratio x,y,z > 3 for O4 8.75 Check

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Ca1 Constrained at 0.3333 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na1 Constrained at 0.6667 Check

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

PLAT432_ALERT_2_G Short Inter X...Y Contact O1 ..C2 . 2.54 Ang.

x-y,x,1/2+z = 6_555 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact O2 ..C3 . 2.94 Ang.

1+x-y,x,1/2+z = 6_655 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact C1 ..C1 . 3.06 Ang.

x-y,x,-1/2+z = 6_554 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact C1 ..C1 . 3.06 Ang.

x-y,x,1/2+z = 6_555 Check

PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 5.75 Ratio

PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !

PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 4 Units

PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ 4 Units

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

- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
- 1 ALERT type 3 Indicator that the structure quality may be low
- 14 ALERT type 4 Improvement, methodology, query or suggestion
- 4 ALERT type 5 Informative message, check

Datablock: p5

Bond precision: O- C = 0.0090 A

Wavelength=0.41122

Cell:	a=10.194(2)	b=10.194(2)	c=6.092(2)
	alpha=90	beta=90	gamma=120
Temperature:	293 K		

	Calculated	Reported
Volume	548.3(3)	548.2(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.067	3.067
Z	2	2
Mu (mm-1)	0.471	0.464
F000	504.0	504.0
F000'	504.79	
h, k, lmax	17, 17, 10	17, 13, 6
Nref	1172[628]	514
Tmin, Tmax	0.978, 0.991	
Tmin'	0.973	

Correction method= Not given

Data completeness= 0.82/0.44 Theta(max)= 21.220

R(reflections)= 0.0311(474)

wR2(reflections)=
0.0750(514)

S = 1.259

Npar= 51

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

PLAT027_ALERT_3_A _diffn_reflths_theta_full value (too) Low	11.83 Degree
PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low .	0.720 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	20.32 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	20.32 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	33.86 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang)	03 Check

● Alert level G

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	1	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122	Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	9.24	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.47	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	8.27	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.64	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	9.46	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1	0.3333	Constrained at Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1	0.6667	Constrained at Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2	2.54	Ang.
	x-y,x,1/2+z =	6_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3	2.94	Ang.
	1+x-y,x,1/2+z =	6_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1	3.05	Ang.
	x-y,x,-1/2+z =	6_554	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1	3.05	Ang.
	x-y,x,1/2+z =	6_555	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	5.75	Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	4	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	4	Units

- 2 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
14 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check
-

Datablock: p6

Bond precision: O- C = 0.0070 A Wavelength=0.41122

Cell: a=10.166(2) b=10.166(2) c=6.066(2)
alpha=90 beta=90 gamma=120

Temperature: 293 K

	Calculated	Reported
Volume	542.9(3)	542.9(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.098	3.097
Z	2	2
Mu (mm-1)	0.475	0.468
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	17,16,6
Nref	1174[629]	524
Tmin,Tmax	0.978,0.991	0.667,1.000
Tmin'	0.972	

Correction method= # Reported T Limits: Tmin=0.667 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.83/0.45 Theta(max)= 21.290

R(reflections)= 0.0267(495)

wR2(reflections)=
0.0669(524)

S = 1.400

Npar= 51

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.690 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density	2.19 Report
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	20.88 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	20.88 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	27.85 Check

Alert level G

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	1	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122	Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	8.95	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	6.82	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	7.96	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.59	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	8.68	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667	Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.54	Ang.
	x-y,x,1/2+z =	6_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.92	Ang.
	1+x-y,x,1/2+z =	6_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.03	Ang.
	x-y,x,-1/2+z =	6_554	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.03	Ang.
	x-y,x,1/2+z =	6_555	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.00	Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	4	Units

-
- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
23 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 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
-

Datablock: p7

Bond precision:	O- C = 0.0080 A	Wavelength=0.41122
Cell:	a=10.137(2)	b=10.137(2)
	alpha=90	beta=90
		gamma=120
Temperature:	293 K	

	Calculated	Reported
Volume	537.9(3)	537.9(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.126	3.126
Z	2	2
Mu (mm-1)	0.480	0.473
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	17,13,6
Nref	1172[628]	507
Tmin,Tmax	0.978,0.991	
Tmin'	0.972	

Correction method= Not given

Data completeness= 0.81/0.43

Theta(max)= 21.360

R(reflections)= 0.0324(481)

wR2(reflections)=
0.0817(507)

S = 1.375

Npar= 50

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.670 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro Please Do !
 PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit P 6c;-2c Check
 PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1 19.08 Check
 PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1 19.08 Check
 PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2 33.79 Check
 PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1 Check
 C3

Alert level G

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

1 Info

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	9.21 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.55 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	8.26 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.96 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	8.94 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293 (K) Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293 (K) Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.54 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.91 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.02 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.02 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.00 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	4 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	4 Units

1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: p8

Bond precision:	O- C = 0.0070 A	Wavelength=0.41122
Cell:	a=10.110 (2)	b=10.110 (2) c=6.013 (2)
	alpha=90	beta=90 gamma=120
Temperature:	293 K	

	Calculated	Reported
Volume	532.3(3)	532.3(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.159	3.159
Z	2	2
Mu (mm-1)	0.485	0.478
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	17,16,5
Nref	1168[626]	501
Tmin,Tmax	0.977,0.990	0.925,1.000
Tmin'	0.972	

Correction method= # Reported T Limits: Tmin=0.925 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.80/0.43 Theta(max)= 21.420

R(reflections)= 0.0234(478)

wR2(reflections)=
0.0596(501)

S = 1.240

Npar= 51

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.690 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro Please Do !
 PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit P 6c;-2c Check
 PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1 19.33 Check
 PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1 19.33 Check
 PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2 27.76 Check

Alert level G

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

1 Info

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	9.25 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	6.86 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	7.57 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.55 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	8.33 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.51 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.90 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.01 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.01 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.00 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5 Units

-
- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 23 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 ALERT type 2 Indicator that the structure model may be wrong or deficient
 1 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
-

Datablock: p9

Bond precision:	O- C = 0.0080 A	Wavelength=0.41122
Cell:	a=10.086(2)	b=10.086(2) c=5.995(2)
	alpha=90	beta=90 gamma=120
Temperature:	293 K	

	Calculated	Reported
Volume	528.2(3)	528.1(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.184	3.184
Z	2	2
Mu (mm-1)	0.489	0.481
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	17,13,5
Nref	1170[627]	492
Tmin,Tmax	0.977,0.990	
Tmin'	0.972	

Correction method= Not given

Data completeness= 0.78/0.42 Theta(max)= 21.480

R(reflections)= 0.0294(467) wR2(reflections)=
0.0715(492)

S = 1.243 Npar= 51

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.670 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	19.02 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	19.02 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	33.68 Check

Alert level G

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	1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..	Please Check

PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	9.19 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.06 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	8.23 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.94 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	8.92 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.51 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.89 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.00 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.00 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.00 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	4 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5 Units

-
- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 24 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 ALERT type 2 Indicator that the structure model may be wrong or deficient
 1 ALERT type 3 Indicator that the structure quality may be low
 14 ALERT type 4 Improvement, methodology, query or suggestion
 4 ALERT type 5 Informative message, check
-

Datablock: p10

Bond precision:	O- C = 0.0080 A	Wavelength=0.41122
Cell:	a=10.061(2)	b=10.061(2) c=5.975(2)
	alpha=90	beta=90 gamma=120
Temperature:	293 K	

	Calculated	Reported
Volume	523.8(3)	523.8(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.211	3.211
Z	2	2
Mu (mm-1)	0.493	0.485
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	17,13,5
Nref	1128[605]	494
Tmin,Tmax	0.977,0.990	
Tmin'	0.971	

Correction method= Not given

Data completeness= 0.82/0.44

Theta(max)= 21.170

R(reflections)= 0.0306(472)

wR2(reflections)=
0.0814(494)

S = 1.397

Npar= 51

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.690 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	20.19 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	20.19 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	35.63 Check

Alert level G

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	1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..	Please Check

PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	8.91 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	6.99 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	8.68 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.94 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	9.40 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.51 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.86 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.99 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.99 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.00 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	4 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5 Units

-
- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
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24 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check
-

Datablock: p11

Bond precision:	O- C = 0.0080 A	Wavelength=0.41122
Cell:	a=10.037(2)	b=10.037(2) c=5.946(2)
	alpha=90	beta=90 gamma=120
Temperature:	293 K	

	Calculated	Reported
Volume	518.8(3)	518.7(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.241	3.242
Z	2	2
Mu (mm-1)	0.498	0.490
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	15,12,5
Nref	1124[603]	482
Tmin,Tmax	0.977,0.990	0.930,1.000
Tmin'	0.971	

Correction method= # Reported T Limits: Tmin=0.930 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.80/0.43 Theta(max)= 21.230

R(reflections)= 0.0284(467)

wR2(reflections)=
0.0703(482)

S = 1.476

Npar= 46

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.670 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	18.96 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	18.96 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	33.57 Check
PLAT201_ALERT_2_C Isotropic non-H Atoms in Main Residue(s) Occ>0.5 O3	1 Report
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang)	O3 Check

Alert level G

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	1	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122	Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	9.48	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.50	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	8.20	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	6.71	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	9.16	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667	Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2	2.50	Ang.
	x-y,x,1/2+z =	6_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3	2.85	Ang.
	1+x-y,x,1/2+z =	6_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1	2.97	Ang.
	x-y,x,-1/2+z =	6_554	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1	2.97	Ang.
	x-y,x,1/2+z =	6_555	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	6.00	Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2	Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	5	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5	Units

1 **ALERT level A** = Most likely a serious problem - resolve or explain
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7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
25 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
5 ALERT type 5 Informative message, check

Datablock: p12

Bond precision: O- C = 0.0070 A Wavelength=0.41122

Cell: a=10.016(2) b=10.016(2) c=5.928(2)
alpha=90 beta=90 gamma=120

Temperature: 293 K

	Calculated	Reported
Volume	515.0(3)	515.0(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.265	3.265
Z	2	2
Mu (mm-1)	0.501	0.494
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	17,15,5
Nref	1126[604]	487
Tmin,Tmax	0.977,0.990	0.953,1.000
Tmin'	0.971	

Correction method= # Reported T Limits: Tmin=0.953 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.81/0.43 Theta(max)= 21.290

R(reflections)= 0.0237(468)

wR2(reflections)=
0.0568(487)

S = 1.236

Npar= 51

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.670 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	19.24 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	19.24 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	27.62 Check

Alert level G

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

1 Info

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	9.21 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.28 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	8.07 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.92 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	9.86 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293 (K) Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293 (K) Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.49 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.83 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.96 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.96 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.00 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5 Units

1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check

Datablock: p13

Bond precision:	O- C = 0.0080 A	Wavelength=0.41122
Cell:	a=9.992 (2)	b=9.992 (2)
	alpha=90	gamma=120
Temperature:	293 K	

ABSMU01_ALERT_1_G Calculation of expt1 absorpt correction mu

not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122	Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	8.87	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.39	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	7.49	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.91	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	9.36	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667	Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.49	Ang.
	x-y,x,1/2+z =	6_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.84	Ang.
	1+x-y,x,1/2+z =	6_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.95	Ang.
	x-y,x,-1/2+z =	6_554	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.95	Ang.
	x-y,x,1/2+z =	6_555	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.00	Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	5	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5	Units

-
- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
14 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check
-

Datablock: p14

Bond precision: O- C = 0.0080 A Wavelength=0.41122

Cell: a=9.969(2) b=9.969(2) c=5.886(2)
 alpha=90 beta=90 gamma=120

Temperature: 293 K

	Calculated	Reported
Volume	506.6(3)	506.6(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.320	3.319
Z	2	2
Mu (mm-1)	0.509	0.502
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	17,12,5
Nref	1122[602]	467
Tmin,Tmax	0.976,0.990	
Tmin'	0.970	

Correction method= Not given

Data completeness= 0.78/0.42

Theta(max)= 21.400

R(reflections)= 0.0325(451)

wR2(reflections)=
0.0783(467)

S = 1.325

Npar= 51

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.670 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	18.89 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	18.89 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	33.46 Check

Alert level G

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	1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..	Please Check

PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	9.12 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.38 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	7.59 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.90 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	8.36 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.48 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.81 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.94 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.94 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.50 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	5 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5 Units

-
- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 24 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 ALERT type 2 Indicator that the structure model may be wrong or deficient
 1 ALERT type 3 Indicator that the structure quality may be low
 14 ALERT type 4 Improvement, methodology, query or suggestion
 4 ALERT type 5 Informative message, check
-

Datablock: p15

Bond precision:	O- C = 0.0070 A	Wavelength=0.41122
Cell:	a=9.952 (2)	b=9.952 (2) c=5.874 (2)
	alpha=90	beta=90 gamma=120
Temperature:	293 K	

	Calculated	Reported
Volume	503.8(3)	503.9(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.338	3.338
Z	2	2
Mu (mm-1)	0.512	0.505
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	15,12,5
Nref	1120[601]	470
Tmin,Tmax	0.976,0.990	0.918,1.000
Tmin'	0.970	

Correction method= # Reported T Limits: Tmin=0.918 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.78/0.42 Theta(max)= 21.440

R(reflections)= 0.0252(454)

wR2(reflections)=
0.0593(470)

S = 1.277

Npar= 51

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.660 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	20.66 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	20.66 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	27.54 Check

Alert level G

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

1 Info

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	8.85 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.72 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	7.87 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.90 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	8.85 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293 (K) Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293 (K) Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.47 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.80 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.94 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.94 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.50 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2 Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	5 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5 Units

-
- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
25 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
5 ALERT type 5 Informative message, check
-

Datablock: p16

Bond precision:	O- C = 0.0070 A	Wavelength=0.41122
Cell:	a=9.931(2)	b=9.931(2)
	alpha=90	beta=90
		gamma=120
Temperature:	293 K	

	Calculated	Reported
Volume	500.0(3)	500.0(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.363	3.363
Z	2	2
Mu (mm-1)	0.516	0.508
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	17,12,5
Nref	1048[564]	465
Tmin,Tmax	0.976,0.990	0.877,1.000
Tmin'	0.970	

Correction method= # Reported T Limits: Tmin=0.877 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.82/0.44 Theta(max)= 21.020

R(reflections)= 0.0244(449)

wR2(reflections)=
0.0567(465)

S = 1.218

Npar= 51

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.670 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	20.63 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	20.63 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	29.47 Check

Alert level G

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

1 Info

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	8.84 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.71 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	8.04 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.89 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	9.43 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293 (K) Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293 (K) Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.47 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.79 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.93 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.93 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.75 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	5 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5 Units

1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check

Datablock: p17

Bond precision:	O- C = 0.0070 A	Wavelength=0.41122
Cell:	a=9.910 (2)	b=9.910 (2)
	alpha=90	gamma=120
Temperature:	293 K	

	Calculated	Reported
Volume	495.9(3)	495.9(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.391	3.391
Z	2	2
Mu (mm-1)	0.520	0.513
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	17,15,5
Nref	1048[564]	464
Tmin,Tmax	0.976,0.990	0.790,1.000
Tmin'	0.970	

Correction method= # Reported T Limits: Tmin=0.790 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.82/0.44 Theta(max)= 21.070

R(reflections)= 0.0241(447)

wR2(reflections)=
0.0606(464)

S = 1.283

Npar= 51

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.670 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1	22.06 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1	22.06 Check
PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2	31.38 Check

Alert level G

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 1 Info

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	9.41 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.56 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	8.33 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	6.28 Check
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3 Note
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.45 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.79 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.91 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.91 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.75 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5 Units

1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check

Datablock: p18

Bond precision:	O- C = 0.0070 A	Wavelength=0.41122
Cell:	a=9.889(2)	b=9.889(2)
	alpha=90	gamma=120
Temperature:	293 K	

	Calculated	Reported
Volume	492.6(3)	492.6(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.414	3.414
Z	2	2
Mu (mm-1)	0.524	0.516
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	15,17,5
Nref	1040[560]	458
Tmin,Tmax	0.976,0.990	0.807,1.000
Tmin'	0.970	

Correction method= # Reported T Limits: Tmin=0.807 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.82/0.44 Theta(max)= 21.110

R(reflections)= 0.0258(442)

wR2(reflections)=
0.0630(458)

S = 1.369

Npar= 51

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.650 Why?

Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro Please Do !
 PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit P 6c;-2c Check
 PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1 20.58 Check
 PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1 20.58 Check
 PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA2 29.41 Check

Alert level G

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

1 Info

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	8.82 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.14 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	7.84 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.88 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	9.41 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293 (K) Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293 (K) Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.45 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.78 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.91 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.91 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.75 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5 Units

1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check

Datablock: p19

Bond precision:	O- C = 0.0200 A	Wavelength=0.41122
Cell:	a=9.873(2)	b=9.873(2)
	alpha=90	gamma=120
Temperature:	293 K	

	Calculated	Reported
Volume	489.5(3)	489.6(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.435	3.435
Z	2	2
Mu (mm-1)	0.527	0.519
F000	504.0	504.0
F000'	504.79	
h,k,lmax	17,17,10	17,15,5
Nref	1040[560]	465
Tmin,Tmax	0.975,0.990	0.778,1.000
Tmin'	0.969	

Correction method= # Reported T Limits: Tmin=0.778 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.83/0.45 Theta(max)= 21.150

R(reflections)= 0.0381(450)

wR2(reflections)=
0.1920(465)

S = 4.108

Npar= 40

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.670 Why?

Alert level B

GOODF01_ALERT_2_B The least squares goodness of fit parameter lies
outside the range 0.60 <> 4.00
Goodness of fit given = 4.108

Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -1.810
Test value = -1.500

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT034_ALERT_1_C	No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	1.62 eA-3
PLAT098_ALERT_2_C	Large Reported Min. (Negative) Residual Density	-1.81 eA-3
PLAT127_ALERT_1_C	Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C	max(sig)/min(sig) ratio x,y,z > 3 for NA1	18.07 Check
PLAT160_ALERT_4_C	max(sig)/min(sig) ratio x,y,z > 3 for CA1	18.07 Check
PLAT160_ALERT_4_C	max(sig)/min(sig) ratio x,y,z > 3 for CA2	26.10 Check
PLAT201_ALERT_2_C	Isotropic non-H Atoms in Main Residue(s) Occ>0.5	3 Report
	O2 O3 C2	

Alert level G

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	1 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	7.83 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.34 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	9.79 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	4.70 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	9.79 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.45 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.79 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.90 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.90 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.75 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5 Units

-
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- 9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check
-

	Calculated	Reported
Volume	487.2(3)	487.1(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	3.452	3.452
Z	2	2
Mu (mm-1)	0.530	0.522
F000	504.0	504.0
F000'	504.79	
h,k,lmax	16,16,9	15,12,5
Nref	979[527]	476
Tmin,Tmax	0.975,0.990	0.749,1.000
Tmin'	0.969	

```
Data completeness= 0.90/0.49          Theta(max)= 20.720
R(reflections)= 0.0237( 460)          wR2(reflections)=
S = 1.284                             0.0556( 476)
Npar= 51
```

 **Alert level A**

PLAT027_ALERT_3_A _diffn_reflths_theta_full	value (too) Low	13.24 Degree
PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full	value Low .	0.700 Why?

● Alert level C

PLAT034_ALERT_1_C	No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT127_ALERT_1_C	Implicit Hall Symbol Inconsistent with Explicit	P 6c;-2c Check
PLAT160_ALERT_4_C	max(sig)/min(sig) ratio x,y,z > 3 for NA1	19.07 Check
PLAT160_ALERT_4_C	max(sig)/min(sig) ratio x,y,z > 3 for CA1	19.07 Check
PLAT160_ALERT_4_C	max(sig)/min(sig) ratio x,y,z > 3 for CA2	27.38 Check

● Alert level G

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	1 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122 Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	9.13 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.22 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	8.00 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.87 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	8.22 Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667 Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.44 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C3 .	2.77 Ang.
	1+x-y,x,1/2+z =	6_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.89 Ang.
	x-y,x,-1/2+z =	6_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	2.89 Ang.
	x-y,x,1/2+z =	6_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	6.75 Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	4 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	4 Units

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Bond precision: O- C = 0.0080 A

Wavelength=0.41122

Cell: a=10.379(2) b=10.379(2) c=6.266(2)
alpha=90 beta=90 gamma=120
Temperature: 293 K

	Calculated	Reported
Volume	584.6(3)	584.6(2)
Space group	P 63 m c	P 63 m c
Hall group	P 6c -2c	P 6c;-2c
Moiety formula	C3 O9, 2(C O3), 4(Ca), 2(Na)	?
Sum formula	C5 Ca4 Na2 O15	C5 Ca4 Na2 O15
Mr	506.35	506.30
Dx, g cm-3	2.877	2.877
Z	2	2
Mu (mm-1)	0.442	0.435
F000	504.0	504.0
F000'	504.79	
h,k,lmax	18,18,11	18,16,6
Nref	1285[687]	535
Tmin,Tmax	0.979,0.991	0.929,1.000
Tmin'	0.974	

Correction method= # Reported T Limits: Tmin=0.929 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.78/0.42

Theta(max)= 21.430

R(reflections)= 0.0282(491)

wR2(reflections)=
0.0704(535)

S = 1.215

Npar= 51

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low .

0.670 Why?



Alert level C

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro

Please Do !

PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit

P 6c;-2c Check

PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for NA1

18.11 Check

PLAT160_ALERT_4_C max(sig)/min(sig) ratio x,y,z > 3 for CA1

18.11 Check

PLAT160_ALERT_4_C	max(sig)/min(sig) ratio x,y,z > 3 for CA2	30.19	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)	03	Check



Alert level G

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	1	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is NOT Cu,Ga,Mo,Ag,In Ka	0.41122	Ang.
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O1	8.78	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2	7.76	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O2	7.33	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O3	5.37	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for O4	9.06	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.6667	Check
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C2 .	2.59	Ang.
	x-y,x,1/2+z =	6_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.13	Ang.
	x-y,x,-1/2+z =	6_554	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C1 .	3.13	Ang.
	x-y,x,1/2+z =	6_555	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	4.75	Ratio
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	5	Units

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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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.











































