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Caesium sodium bis(formate)

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The title compound, $CsNa(CHO_2)_2$, was obtained from the crystallization of caesium formate in a glass container. It has a complex structure, with sodium ions octahedrally coordinated and caesium ions irregularly eight-coordinated by the formate O atoms. One Cs cation and four formate C atoms have site symmetry *m* and one Na cation has site symmetry $\overline{1}$, resulting in the unusual situation of $Z = 12$ for an orthorhombic structure.

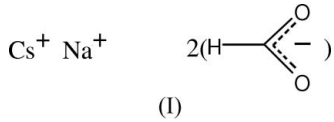
Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(O–C) = 0.004 Å
R factor = 0.034
wR factor = 0.090
Data-to-parameter ratio = 19.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

During a study of the crystal structure of caesium formate (Wilson *et al.*, 2006), it was found that, if the crystallization of caesium formate by diffusion is carried out in a glass container, the crystals formed are of a mixed caesium sodium salt, $CsNa(C_2HO_2)_2$, (I).



(I)

The sodium ions were identified from the crystal structure analysis. After initial location of the Cs atoms, the chemical identity of two medium height electron-density peaks was tested by refinement. Only the assignment of Na to the peaks both satisfied stoichiometric requirements and gave satisfactory displacement parameters (as well as providing much the best R value). It is inferred that their source is the glass vials used for crystallization, and it has been shown (Wilson *et al.*, 2006) that recrystallization from polythene vials gives unchanged caesium formate. Similar extraction of sodium cations by formate solutions has been reported by Robinet *et al.* (2004).

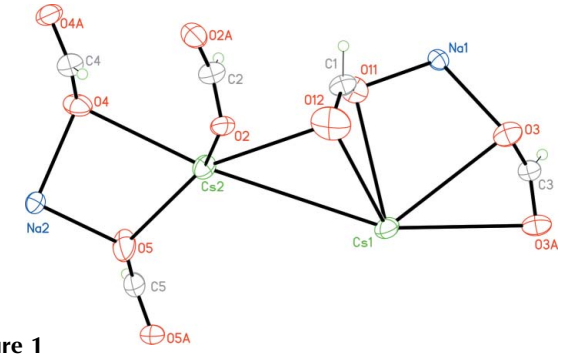


Figure 1
View of the asymmetric unit of (I) (with formate ions completed by symmetry), showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). Cs, H, Na and O atoms are green (large), green (small), blue and red, respectively. [Symmetry codes: x, $-\frac{1}{2} - y$, z (for O2A and O4A); x, $\frac{1}{2} - y$, z (for O3A and O5A)].

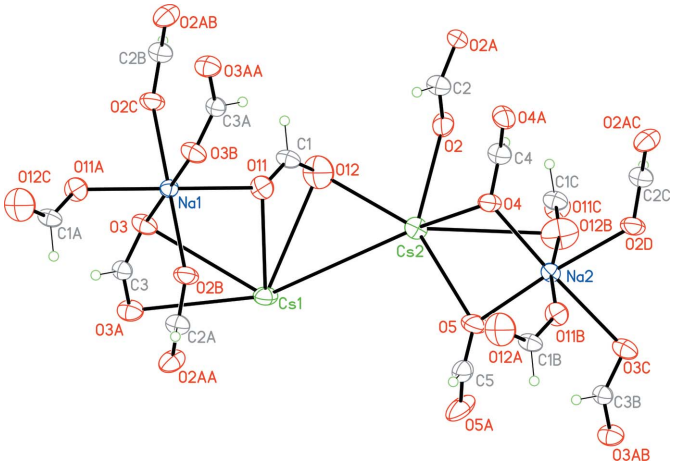


Figure 2
The structure with the Na ion coordination completed. Atom colouring as in Fig. 1. [Symmetry codes: $x, -\frac{1}{2}-y, z$ (O2A and O4A); $x, \frac{1}{2}-y, z$ (O3A, O5A, O11A, O12A and C1A); $2-x, -y, 1-z$ (C4A, O4B, O5B and C5A); $2-x, \frac{1}{2}-y, 1-z$ (O4AA and O5AA); $\frac{1}{2}+x, y, \frac{3}{2}-z$ (O11B, O12B and C1B)].

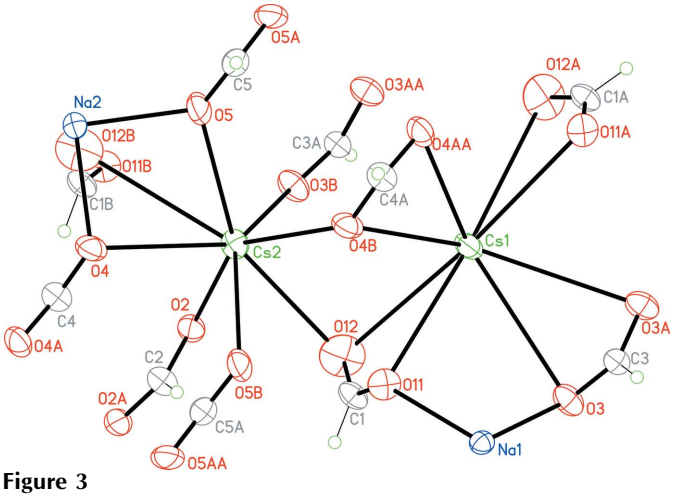


Figure 3
The structure with the Cs ion coordination completed. Atom colouring as in Fig. 1. [Symmetry codes: $x, -\frac{1}{2}-y, z$ (O2A and O4A); $x, \frac{1}{2}-y, z$ (O3A and O5A); $\frac{1}{2}+x, y, \frac{3}{2}-z$ (O11A, C1, O12C, O12B, C1C, O11C, O2D and C2C); $\frac{1}{2}+x, -1+y, \frac{3}{2}-z$ (O2C and C2B); $\frac{3}{2}-x, -y, -\frac{1}{2}-z$ (O2B and C2A); $1-x, -y, 1-z$ (O3B and C3A); $2-x, -y, 1-z$ (O11B, C1B and O12A); $\frac{3}{2}-x, -y, -\frac{1}{2}-z$ (O2AA); $-\frac{1}{2}+x, -\frac{1}{2}-y, \frac{3}{2}-z$ (O2AB); $\frac{1}{2}+x, -\frac{1}{2}-y, \frac{3}{2}-z$ (O2AC); $\frac{1}{2}+x, \frac{3}{2}-y, \frac{1}{2}-z$ (O3AB); $1-x, -\frac{1}{2}+y, 1-z$ (O3AA); $1+x, y, z$ (O3C and C3B)].

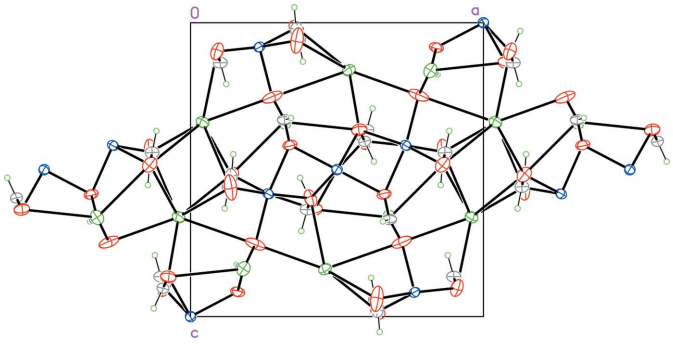


Figure 4
The packing, viewed down the *b* axis. Atom colouring as in Fig. 1.

In the structure of (I) (Fig. 1), both Na ions are octahedrally coordinated, with Na—O distances (Table 1) in the range 2.243 (4)–2.678 (3) Å (Fig. 2). The coordination of the Cs ions (Fig. 3) is best regarded as eight-coordinate, with Cs1 having square-antiprismatic geometry and Cs2 a less regular arrangement of ligand O atoms [Cs—O = 3.007 (3)–3.550 (4) Å], but with additional O atoms within 0.3 Å. The overall packing (Fig. 4) can be described as including chains of cations bridged by formate ions.

Experimental

AR standard caesium formate (Aldrich) was dissolved in a minimum volume of methanol in a glass vial. This (open) container was then placed inside a larger vial containing a small amount of 1-butanol and the whole system sealed immediately. Crystallization proceeded with occasional swirling of the suspension over a two-week period.

Crystal data

$CsNa(CHO_2)_2$
$M_r = 245.94$
Orthorhombic, *Pnma*
$a = 12.5812\ (3)$ Å
$b = 11.0509\ (3)$ Å
$c = 12.6024\ (3)$ Å
$V = 1752.16\ (8)$ Å^3
$Z = 12$
$D_x = 2.797$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8192 reflections
$\theta = 3$–25°
$\mu = 6.34$ mm^{-1}
$T = 180\ (2)$ K
Block, colourless
0.20 × 0.20 × 0.15 mm

Data collection

Siemens SMART diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.202$, $T_{max} = 0.387$
10798 measured reflections
2324 independent reflections
1867 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 29.1^\circ$
$h = -15 \rightarrow 16$
$k = -15 \rightarrow 14$
$l = -14 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.090$
$S = 1.03$
2324 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 1.59$ e Å^{-3}
$\Delta\rho_{min} = -1.59$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0039 (3)

Table 1
Selected bond lengths (Å).

Cs1—O11	3.193 (3)	Cs2—O12^{iv}	3.516 (4)
Cs1—O12	3.294 (4)	Cs2—O2	3.550 (4)
Cs1—O4^{i}	3.389 (3)	Na1—O11	2.298 (3)
Cs1—O3	3.441 (3)	Na1—O2^{ii}	2.350 (3)
Cs1—O2^{ii}	3.642 (4)	Na1—O3	2.553 (3)
Cs2—O4^{iii}	3.007 (3)	Na2—O12^{iv}	2.243 (4)
Cs2—O5	3.015 (3)	Na2—O11^{iii}	2.313 (3)
Cs2—O3^{iv}	3.027 (3)	Na2—O5	2.354 (4)
Cs2—O12	3.206 (4)	Na2—O4	2.416 (3)
Cs2—O4	3.386 (3)	Na2—O2^{iv}	2.443 (3)
Cs2—O5^{iii}	3.510 (5)	Na2—O3^{v}	2.678 (3)

Symmetry codes: (i) $-x+2, y+\frac{1}{2}, -z+1$; (ii) $-x+\frac{3}{2}, -y, z-\frac{1}{2}$; (iii) $-x+2, -y, -z+1$; (iv) $x+\frac{1}{2}, y, -z+\frac{3}{2}$; (v) $x+1, y, z$.

H atoms were placed in calculated positions and refined using a riding model [C—H = 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The highest and lowest peaks on the difference map are all close to the Cs positions.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Orthorhombic, *Pnma*
Hall symbol: -P 2ac 2n
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$b = 11.0509$ (3) Å
$c = 12.6024$ (3) Å
$V = 1752.16$ (8) Å^3
$Z = 12$
$F(000) = 1344$
$D_x = 2.797$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8192 reflections
$\theta = 3$–25°
$\mu = 6.34$ mm^{-1}
$T = 180$ K
Block, colourless
0.20 × 0.20 × 0.15 mm

Data collection

Siemens SMART diffractometer
Radiation source: normal-focus sealed tube
Graphite monochromator
Detector resolution: 8.192 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.202$, $T_{max} = 0.387$
10798 measured reflections
2324 independent reflections
1867 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 29.1°$, $\theta_{min} = 2.3°$
$h = -15 \rightarrow 16$
$k = -15 \rightarrow 14$
$l = -14 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.090$
$S = 1.03$
2324 reflections
119 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 1.59$ e Å^{-3}
$\Delta\rho_{min} = -1.59$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0039 (3)

Special details

Experimental. The temperature of the crystal was controlled using the Oxford Cryosystems Cryostream Cooler (Cosier & Glazer, 1986). The data collection nominally covered over a hemisphere of reciprocal space, by a combination of three sets of exposures with different φ angles for the crystal; each 10 s exposure covered 0.3° in ω. The crystal-to-detector distance was 5.0 cm. Coverage of the unique set is over 97% complete to at least 26° in θ. Crystal decay was found to be negligible by repeating the initial frames at t data collection and analyzing the duplicate reflections.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cs1	0.68069 (3)	0.2500	0.66245 (3)	0.03135 (14)
Cs2	0.95906 (2)	0.00768 (2)	0.66158 (2)	0.02852 (12)
Na1	0.5000	0.0000	0.5000	0.0219 (4)
Na2	1.26514 (12)	−0.00181 (12)	0.58246 (11)	0.0216 (3)
C1	0.6791 (3)	−0.0706 (4)	0.6696 (3)	0.0272 (9)
H1A	0.6570	−0.1525	0.6762	0.033*
O11	0.6608 (3)	−0.0238 (3)	0.5840 (2)	0.0320 (7)
O12	0.7211 (3)	−0.0284 (4)	0.7467 (3)	0.0585 (11)
C2	0.8986 (5)	−0.2500	0.8641 (5)	0.0286 (12)
H2A	0.8783	−0.2500	0.7914	0.034*
O2	0.9093 (2)	−0.1489 (3)	0.9025 (3)	0.0378 (8)
C3	0.4057 (4)	0.2500	0.5962 (4)	0.0237 (11)
H3A	0.3742	0.2500	0.5277	0.028*
O3	0.4236 (3)	0.1483 (3)	0.6353 (2)	0.0330 (7)
C4	1.1312 (5)	−0.2500	0.5582 (5)	0.0300 (12)
H4A	1.1165	−0.2500	0.6321	0.036*
O4	1.1394 (2)	−0.1491 (3)	0.5170 (3)	0.0355 (7)
C5	1.1395 (5)	0.2500	0.5225 (6)	0.0334 (13)
H5A	1.1458	0.2500	0.4474	0.040*
O5	1.1363 (3)	0.1506 (3)	0.5604 (4)	0.0616 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs1	0.0343 (2)	0.0192 (2)	0.0405 (2)	0.000	0.00677 (16)	0.000
Cs2	0.03137 (19)	0.02912 (18)	0.02506 (18)	0.00280 (10)	0.00471 (10)	−0.00124 (9)
Na1	0.0216 (11)	0.0223 (11)	0.0217 (11)	−0.0020 (8)	−0.0006 (9)	0.0033 (8)
Na2	0.0230 (8)	0.0227 (8)	0.0192 (8)	0.0023 (6)	0.0031 (6)	0.0016 (5)
C1	0.040 (2)	0.020 (2)	0.0210 (19)	0.0007 (16)	−0.0003 (16)	0.0029 (14)
O11	0.0387 (18)	0.0389 (17)	0.0183 (14)	−0.0030 (13)	−0.0049 (12)	0.0040 (12)
O12	0.077 (3)	0.070 (3)	0.0280 (19)	−0.007 (2)	−0.0244 (19)	−0.0006 (17)

C2	0.039 (3)	0.025 (3)	0.022 (3)	0.000	0.000 (2)	0.000
O2	0.0317 (16)	0.0254 (16)	0.056 (2)	0.0023 (12)	−0.0121 (14)	−0.0159 (14)
C3	0.028 (3)	0.023 (3)	0.020 (3)	0.000	−0.002 (2)	0.000
O3	0.0466 (18)	0.0256 (16)	0.0268 (15)	0.0034 (13)	−0.0036 (13)	0.0048 (12)
C4	0.037 (3)	0.027 (3)	0.026 (3)	0.000	−0.001 (2)	0.000
O4	0.0402 (16)	0.0232 (15)	0.0433 (17)	−0.0059 (12)	−0.0114 (14)	0.0087 (13)
C5	0.024 (3)	0.031 (3)	0.046 (4)	0.000	0.004 (3)	0.000
O5	0.0313 (18)	0.0275 (18)	0.126 (4)	0.0071 (14)	0.013 (2)	0.028 (2)

Geometric parameters (Å, º)

Cs1—O11	3.193 (3)	Na2—O3^{viii}	2.678 (3)
Cs1—O11^{i}	3.193 (3)	C1—O12	1.201 (5)
Cs1—O12	3.294 (4)	C1—O11	1.217 (4)
Cs1—O12^{i}	3.294 (4)	C1—H1A	0.9500
Cs1—O4^{ii}	3.389 (3)	O11—Na2^{iii}	2.313 (3)
Cs1—O4^{iii}	3.389 (3)	O12—Na2^{vii}	2.243 (4)
Cs1—O3	3.441 (3)	O12—Cs2^{vii}	3.516 (4)
Cs1—O3^{i}	3.441 (3)	C2—O2	1.225 (4)
Cs1—O2^{iv}	3.642 (4)	C2—O2^{ix}	1.225 (4)
Cs2—O4^{iii}	3.007 (3)	C2—H2A	0.9500
Cs2—O5	3.015 (3)	O2—Na1^{x}	2.350 (3)
Cs2—O3^{v}	3.027 (3)	O2—Na2^{vii}	2.443 (3)
Cs2—O12	3.206 (4)	O2—Cs1^{x}	3.642 (4)
Cs2—O4	3.386 (3)	C3—O3^{i}	1.248 (4)
Cs2—O5^{iii}	3.510 (5)	C3—O3	1.248 (4)
Cs2—O12^{v}	3.516 (4)	C3—H3A	0.9500
Cs2—O2	3.550 (4)	O3—Na2^{xi}	2.678 (3)
Na1—O11^{vi}	2.298 (3)	O3—Cs2^{vii}	3.027 (3)
Na1—O11	2.298 (3)	C4—O4^{ix}	1.233 (4)
Na1—O2^{vii}	2.350 (3)	C4—O4	1.233 (4)
Na1—O2^{iv}	2.350 (3)	C4—H4A	0.9500
Na1—O3^{vi}	2.553 (3)	O4—Cs2^{iii}	3.007 (3)
Na1—O3	2.553 (3)	O4—Cs1^{iii}	3.389 (3)
Na2—O12^{v}	2.243 (4)	C5—O5^{i}	1.199 (4)
Na2—O11^{iii}	2.313 (3)	C5—O5	1.199 (4)
Na2—O5	2.354 (4)	C5—H5A	0.9500
Na2—O4	2.416 (3)	O5—Cs2^{iii}	3.510 (5)
Na2—O2^{v}	2.443 (3)	O5—Cs1^{v}	3.704 (5)
O11—Cs1—O11^{i}	142.76 (10)	O11^{iii}—Na2—O5	94.74 (14)
O11—Cs1—O12	39.35 (8)	O12^{v}—Na2—O4	94.44 (14)
O11^{i}—Cs1—O12	175.52 (9)	O11^{iii}—Na2—O4	92.12 (12)
O11—Cs1—O12^{i}	175.52 (9)	O5—Na2—O4	89.47 (13)
O11^{i}—Cs1—O12^{i}	39.35 (8)	O12^{v}—Na2—O2^{v}	91.25 (14)
O12—Cs1—O12^{i}	138.13 (12)	O11^{iii}—Na2—O2^{v}	81.55 (11)
O11—Cs1—O4^{ii}	99.06 (7)	O5—Na2—O2^{v}	175.20 (13)
O11^{i}—Cs1—O4^{ii}	62.23 (8)	O4—Na2—O2^{v}	93.69 (12)

O12—Cs1—O4^{ii}	114.79 (9)	O12^{v}—Na2—O3^{viii}	91.51 (14)
O12^{i}—Cs1—O4^{ii}	78.75 (9)	O11^{iii}—Na2—O3^{viii}	81.36 (10)
O11—Cs1—O4^{iii}	62.23 (8)	O5—Na2—O3^{viii}	95.68 (13)
O11^{i}—Cs1—O4^{iii}	99.06 (7)	O4—Na2—O3^{viii}	171.99 (12)
O12—Cs1—O4^{iii}	78.75 (9)	O2^{v}—Na2—O3^{viii}	80.80 (11)
O12^{i}—Cs1—O4^{iii}	114.79 (9)	O12—C1—O11	129.4 (5)
O4^{ii}—Cs1—O4^{iii}	38.40 (10)	O12—C1—H1A	115.3
O11—Cs1—O3	65.55 (8)	O11—C1—H1A	115.3
O11^{i}—Cs1—O3	101.84 (8)	C1—O11—Na1	128.5 (3)
O12—Cs1—O3	82.64 (8)	C1—O11—Na2^{iii}	141.2 (3)
O12^{i}—Cs1—O3	118.82 (9)	Na1—O11—Na2^{iii}	85.57 (10)
O4^{ii}—Cs1—O3	132.00 (7)	C1—O11—Cs1	96.5 (2)
O4^{iii}—Cs1—O3	117.02 (7)	Na1—O11—Cs1	95.91 (10)
O11—Cs1—O3^{i}	101.84 (8)	Na2^{iii}—O11—Cs1	97.64 (10)
O11^{i}—Cs1—O3^{i}	65.55 (8)	C1—O12—Na2^{vii}	159.5 (4)
O12—Cs1—O3^{i}	118.82 (9)	C1—O12—Cs2	100.8 (3)
O12^{i}—Cs1—O3^{i}	82.64 (8)	Na2^{vii}—O12—Cs2	94.24 (12)
O4^{ii}—Cs1—O3^{i}	117.02 (7)	C1—O12—Cs1	92.0 (3)
O4^{iii}—Cs1—O3^{i}	132.00 (7)	Na2^{vii}—O12—Cs1	103.02 (15)
O3—Cs1—O3^{i}	38.13 (10)	Cs2—O12—Cs1	85.41 (10)
O11—Cs1—O2^{iv}	53.60 (7)	C1—O12—Cs2^{vii}	84.1 (3)
O11^{i}—Cs1—O2^{iv}	89.30 (7)	Na2^{vii}—O12—Cs2^{vii}	84.34 (12)
O12—Cs1—O2^{iv}	92.95 (7)	Cs2—O12—Cs2^{vii}	166.34 (15)
O12^{i}—Cs1—O2^{iv}	128.64 (8)	Cs1—O12—Cs2^{vii}	81.69 (10)
O4^{ii}—Cs1—O2^{iv}	73.03 (7)	O2—C2—O2^{ix}	131.5 (6)
O4^{iii}—Cs1—O2^{iv}	60.42 (7)	O2^{ix}—C2—H2A	114.2
O3—Cs1—O2^{iv}	61.21 (7)	O2—C2—H2A	114.2
O3^{i}—Cs1—O2^{iv}	73.66 (7)	C2—O2—Na1^{x}	154.0 (4)
C1—Cs1—O2^{iv}	73.40 (7)	C2—O2—Na2^{vii}	123.8 (4)
C1^{i}—Cs1—O2^{iv}	109.12 (7)	Na1^{x}—O2—Na2^{vii}	81.59 (10)
C3—Cs1—O2^{iv}	59.13 (9)	C2—O2—Cs2	97.2 (3)
O4^{iii}—Cs2—O5	73.48 (10)	Na1^{x}—O2—Cs2	91.15 (10)
O4^{iii}—Cs2—O3^{v}	107.78 (9)	Na2^{vii}—O2—Cs2	82.70 (9)
O5—Cs2—O3^{v}	101.39 (11)	C2—O2—Cs1^{x}	92.4 (3)
O4^{iii}—Cs2—O12	86.02 (9)	Na1^{x}—O2—Cs1^{x}	83.99 (9)
O5—Cs2—O12	153.82 (10)	Na2^{vii}—O2—Cs1^{x}	84.46 (10)
O3^{v}—Cs2—O12	69.11 (9)	Cs2—O2—Cs1^{x}	166.81 (9)
O4^{iii}—Cs2—O4	98.00 (7)	O3^{i}—C3—O3	128.5 (5)
O5—Cs2—O4	62.95 (9)	O3^{i}—C3—H3A	115.8
O3^{v}—Cs2—O4	144.70 (8)	O3—C3—H3A	115.8
O12—Cs2—O4	137.91 (9)	C3—O3—Na1	112.5 (3)
O4^{iii}—Cs2—O5^{iii}	61.43 (8)	C3—O3—Na2^{xi}	108.9 (3)
O5—Cs2—O5^{iii}	100.17 (9)	Na1—O3—Na2^{xi}	73.52 (9)
O3^{v}—Cs2—O5^{iii}	151.55 (8)	C3—O3—Cs2^{vii}	145.4 (3)
O12—Cs2—O5^{iii}	83.43 (9)	Na1—O3—Cs2^{vii}	100.36 (10)
O4—Cs2—O5^{iii}	62.95 (7)	Na2^{xi}—O3—Cs2^{vii}	90.11 (9)
O4^{iii}—Cs2—O12^{v}	133.71 (8)	C3—O3—Cs1	85.1 (3)
O5—Cs2—O12^{v}	60.34 (10)	Na1—O3—Cs1	85.55 (9)

O3^{v}—Cs2—O12^{v}	85.31 (8)	Na2^{xi}—O3—Cs1	157.95 (12)
O12—Cs2—O12^{v}	138.74 (5)	Cs2^{vii}—O3—Cs1	86.87 (8)
O4—Cs2—O12^{v}	59.39 (8)	O4^{ix}—C4—O4	129.3 (6)
O5^{iii}—Cs2—O12^{v}	121.73 (8)	O4^{ix}—C4—H4A	115.4
O4^{iii}—Cs2—O2	145.17 (8)	O4—C4—H4A	115.4
O5—Cs2—O2	138.37 (9)	C4—O4—Na2	121.3 (3)
O3^{v}—Cs2—O2	60.09 (8)	C4—O4—Cs2^{iii}	138.6 (3)
O12—Cs2—O2	59.23 (8)	Na2—O4—Cs2^{iii}	100.07 (10)
O4—Cs2—O2	109.19 (7)	C4—O4—Cs2	100.4 (3)
O5^{iii}—Cs2—O2	112.23 (8)	Na2—O4—Cs2	84.85 (10)
O12^{v}—Cs2—O2	80.15 (7)	Cs2^{iii}—O4—Cs2	82.00 (7)
O11^{vi}—Na1—O11	180.0	C4—O4—Cs1^{iii}	92.2 (3)
O11^{vi}—Na1—O2^{vii}	83.90 (11)	Na2—O4—Cs1^{iii}	90.68 (10)
O11—Na1—O2^{vii}	96.10 (11)	Cs2^{iii}—O4—Cs1^{iii}	86.93 (8)
O11^{vi}—Na1—O2^{iv}	96.10 (11)	Cs2—O4—Cs1^{iii}	167.13 (10)
O11—Na1—O2^{iv}	83.90 (11)	O5^{i}—C5—O5	132.8 (8)
O2^{vii}—Na1—O2^{iv}	180.0	O5—C5—H5A	113.6
O11^{vi}—Na1—O3^{vi}	95.57 (10)	O5^{i}—C5—H5A	113.6
O11—Na1—O3^{vi}	84.43 (10)	C5—O5—Na2	132.8 (4)
O2^{vii}—Na1—O3^{vi}	94.74 (11)	C5—O5—Cs2	132.3 (4)
O2^{iv}—Na1—O3^{vi}	85.26 (11)	Na2—O5—Cs2	94.85 (12)
O11^{vi}—Na1—O3	84.43 (10)	C5—O5—Cs2^{iii}	98.7 (4)
O11—Na1—O3	95.57 (10)	Na2—O5—Cs2^{iii}	88.45 (13)
O2^{vii}—Na1—O3	85.27 (11)	Cs2—O5—Cs2^{iii}	79.83 (9)
O2^{iv}—Na1—O3	94.73 (11)	C5—O5—Cs1^{v}	95.7 (4)
O3^{vi}—Na1—O3	180.0	Na2—O5—Cs1^{v}	89.83 (13)
O12^{v}—Na2—O11^{iii}	170.56 (15)	Cs2—O5—Cs1^{v}	82.42 (10)
O12^{v}—Na2—O5	92.11 (16)	Cs2^{iii}—O5—Cs1^{v}	161.95 (11)

Symmetry codes: (i) x, $-y+1/2$, z; (ii) $-x+2$, $y+1/2$, $-z+1$; (iii) $-x+2$, $-y$, $-z+1$; (iv) $-x+3/2$, $-y$, $z-1/2$; (v) $x+1/2$, y, $-z+3/2$; (vi) $-x+1$, $-y$, $-z+1$; (vii) $x-1/2$, y, $-z+3/2$; (viii) $x+1$, y, z; (ix) x, $-y-1/2$, z; (x) $-x+3/2$, $-y$, $z+1/2$; (xi) $x-1$, y, z.