Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Disodium 4,4′-oxydibenzoate

Yuan Yang,[a] Qi Li[b] and Seik Weng Ng[c]*

[a]School of Physics and Chemistry, Guizhou Normal University, Guiyang, Guizhou 550001, People's Republic of China, [b]College of Chemistry, Beijing Normal University, Beijing 100875, People's Republic of China, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

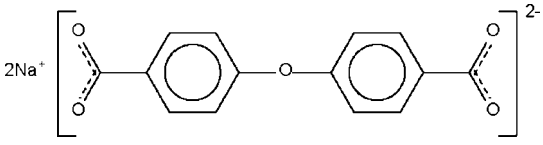
Received 17 July 2008; accepted 30 July 2008

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.043; wR factor = 0.135; data-to-parameter ratio = 7.2.

The crystal structure of the title compound, $2Na^{+}\cdot C_{14}H_8O_5^{2-}$, consists of alternating layers of sodium cations and 4,4′-oxydibenzoate anions; the layers are perpendicular to the a axis, with the distance between the layers of cations (or anions) being half this axial length. The Na atoms are disordered over three sites [occupancies 0.775 (4), 0.781 (6) 0.444 (6)].

Related literature

For the crystal structure of 4,4′-oxybis(benzoic acid), see: Dey & Desiraju (2005); Potts *et al.* (2007).



Experimental

Crystal data

$2Na^{+}\cdot C_{14}H_8O_5^{2-}$ M_r = 302.18
Monoclinic, Cc
a = 29.1091 (4) Å
b = 5.7801 (1) Å
c = 7.6429 (1) Å
β = 92.4420 (1)°
V = 1284.78 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 295 (2) K
0.5 × 0.4 × 0.2 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.888, T_{max} = 1.000
(expected range = 0.857–0.966)
5002 measured reflections
1471 independent reflections
1464 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.135
S = 1.27
1471 reflections
203 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

We thank Beijing Normal University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2752).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dey, A. & Desiraju, G. R. (2005). *Chem. Commun.* pp. 2486–2488.
Potts, S., Bredenkamp, M. W. & Gertenbach, J.-A. (2007). *Acta Cryst.* E**63**, o2887.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2008). *publCIF*. In preparation.

supporting information

Acta Cryst. (2008). E**64**, m1119 [doi:10.1107/S1600536808024331]

Disodium 4,4′-oxydibenzoate

Yuan Yang, Qi Li and Seik Weng Ng

S1. Comment

The crystal structure of disodium 4,4′-oxydibenzoate (Scheme I, Fig. 1) consists of alternating bands of sodium cations and 4,4′-oxydibenzoate anions. The two symmetry-independent sodium atoms over three positions. The lowest occupancy sodium atom is only weakly linked to two oxygen atoms, and probably "rattles" about in the crystal structure.

S2. Experimental

Betaine (0.047 g, 0.4 mmol), 4,4′-oxybis(benzoic acid) (0.103 g, 0.4 mmol) and guanidine hydrochloride (0.076 g, 0.8 mmol) were mixed in a molar ratio 1:1:2. The mixture was dissolved in mixture of ethanol (4 ml), 1 *M* sodium hydroxide (0.5 ml) and water (0.5 ml). Colorless crystals were obtained after about 10 days.

S3. Refinement

The Na1, Na2 and Na3 atoms were refined such that the total occupancy is two.

Carbon bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) 1.2U_{eq}(C).

Friedel pairs were merged as there are no anomalous scatterers.

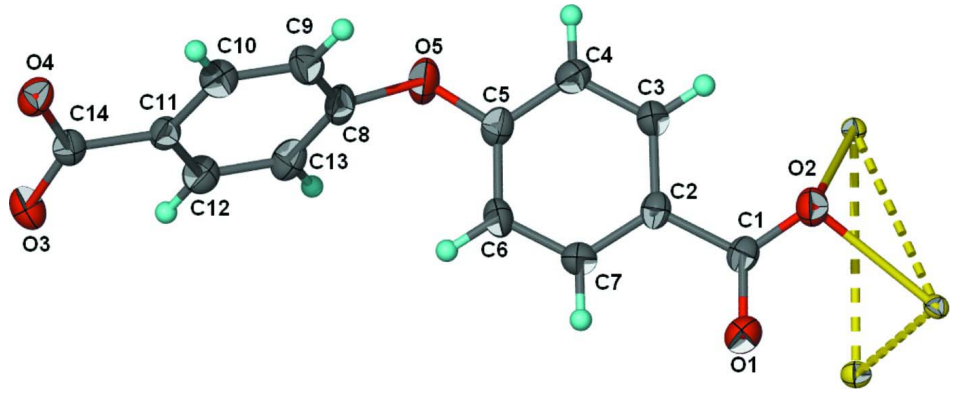


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the asymmetric unit of the title compound; displac ement ellipsoids are set at the 70% probability level. Hydrogeatoms are drawn as spheres of arbitrary radius. The two sodium atoms are disordered over three positions. Dashed lines denote the distances between them.

Disodium 4,4′-oxydibenzoate

Crystal data

$2Na^{+}\cdot C_{14}H_8O_5^{2-}$
$M_r = 302.18$
Monoclinic, *Cc*
$a = 29.1091$ (4) Å
$b = 5.7801$ (1) Å
$c = 7.6429$ (1) Å
$\beta = 92.4420$ (1)°
$V = 1284.78$ (3) Å^3
$Z = 4$
$F(000) = 616$
$D_x = 1.562$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4314 reflections
$\theta = 4.0$–$27.5°$
$\mu = 0.18$ mm^{-1}
$T = 295$ K
Block, colorless
0.5 × 0.4 × 0.2 mm

Data collection

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.888$, $T_{max} = 1.000$
5002 measured reflections
1471 independent reflections
1464 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 27.5°$, $\theta_{min} = 4.1°$
$h = -37\rightarrow37$
$k = -7\rightarrow7$
$l = -9\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.135$
$S = 1.27$
1471 reflections
203 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0883P)^2 + 0.9438P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.79$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.024 (4)

Special details

Experimental. A somewhat large crystal was used in the measurements, but this does not seem to have an adverse efffect on the quality of the diffraction data.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Na1	0.50001 (5)	0.1573 (3)	0.50001 (18)	0.0119 (4)	0.775 (4)
Na2	0.44106 (5)	0.3880 (3)	0.84063 (18)	0.0113 (5)	0.781 (6)
Na3	0.47490 (10)	0.7168 (5)	0.7153 (4)	0.0147 (9)	0.444 (6)
O1	0.53701 (10)	0.4833 (5)	0.9932 (4)	0.0273 (6)	
O2	0.51425 (9)	0.1864 (5)	0.8264 (4)	0.0243 (6)	
O3	0.91491 (10)	0.5648 (5)	0.9768 (4)	0.0279 (6)	
O4	0.92132 (9)	0.1917 (5)	1.0487 (4)	0.0249 (6)	
O5	0.72485 (10)	0.1735 (6)	0.6575 (4)	0.0338 (7)	

C1	0.54493 (12)	0.3222 (6)	0.8891 (5)	0.0199 (7)
C2	0.59376 (12)	0.2835 (6)	0.8364 (4)	0.0199 (7)
C3	0.60419 (13)	0.0883 (6)	0.7386 (5)	0.0234 (7)
H3	0.5812	−0.0182	0.7088	0.028*
C4	0.64896 (13)	0.0513 (7)	0.6849 (5)	0.0250 (7)
H4	0.6559	−0.0793	0.6201	0.030*
C5	0.68284 (12)	0.2121 (7)	0.7296 (5)	0.0230 (7)
C6	0.67343 (13)	0.4048 (7)	0.8307 (5)	0.0251 (8)
H6	0.6966	0.5089	0.8634	0.030*
C7	0.62823 (12)	0.4391 (7)	0.8825 (5)	0.0228 (7)
H7	0.6214	0.5685	0.9488	0.027*
C8	0.76546 (12)	0.2304 (8)	0.7501 (5)	0.0261 (8)
C9	0.78630 (13)	0.0650 (7)	0.8574 (5)	0.0266 (8)
H9	0.7713	−0.0733	0.8792	0.032*
C10	0.82982 (14)	0.1068 (7)	0.9322 (5)	0.0248 (7)
H10	0.8442	−0.0052	1.0026	0.030*
C11	0.85196 (11)	0.3161 (6)	0.9022 (4)	0.0194 (7)
C12	0.82984 (13)	0.4838 (7)	0.7983 (5)	0.0243 (7)
H12	0.8440	0.6256	0.7813	0.029*
C13	0.78638 (13)	0.4407 (7)	0.7192 (5)	0.0264 (7)
H13	0.7719	0.5509	0.6475	0.032*
C14	0.89941 (12)	0.3616 (6)	0.9821 (5)	0.0200 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0114 (7)	0.0098 (7)	0.0144 (7)	0.0005 (5)	−0.0009 (5)	−0.0005 (5)
Na2	0.0119 (8)	0.0094 (7)	0.0127 (8)	−0.0011 (5)	0.0003 (5)	0.0001 (5)
Na3	0.0169 (14)	0.0144 (15)	0.0127 (14)	0.0013 (10)	0.0008 (10)	−0.0004 (10)
O1	0.0230 (11)	0.0294 (14)	0.0299 (15)	0.0020 (11)	0.0043 (10)	−0.0037 (11)
O2	0.0183 (11)	0.0254 (13)	0.0293 (13)	−0.0020 (9)	0.0007 (10)	0.0005 (10)
O3	0.0262 (13)	0.0292 (15)	0.0282 (14)	−0.0081 (11)	−0.0015 (11)	0.0009 (11)
O4	0.0209 (12)	0.0281 (13)	0.0254 (13)	0.0042 (10)	−0.0017 (10)	0.0008 (10)
O5	0.0171 (12)	0.056 (2)	0.0288 (14)	−0.0011 (12)	0.0005 (10)	−0.0141 (13)
C1	0.0181 (15)	0.0215 (15)	0.0200 (15)	0.0019 (12)	0.0015 (12)	0.0039 (12)
C2	0.0165 (15)	0.0228 (16)	0.0204 (15)	0.0011 (12)	−0.0006 (12)	0.0030 (12)
C3	0.0187 (16)	0.0241 (17)	0.0274 (18)	−0.0015 (13)	0.0007 (13)	−0.0029 (13)
C4	0.0223 (17)	0.0260 (17)	0.0267 (17)	0.0035 (15)	0.0008 (13)	−0.0051 (14)
C5	0.0179 (16)	0.0299 (17)	0.0211 (15)	0.0015 (13)	0.0003 (12)	−0.0001 (13)
C6	0.0174 (16)	0.0290 (19)	0.0287 (17)	−0.0044 (13)	−0.0014 (13)	−0.0039 (15)
C7	0.0226 (17)	0.0217 (16)	0.0243 (17)	−0.0001 (13)	0.0016 (13)	−0.0034 (12)
C8	0.0159 (16)	0.039 (2)	0.0232 (17)	−0.0016 (14)	0.0031 (13)	−0.0074 (15)
C9	0.0227 (17)	0.0278 (18)	0.0294 (18)	−0.0069 (14)	0.0037 (14)	−0.0022 (14)
C10	0.0260 (18)	0.0237 (16)	0.0247 (17)	−0.0007 (14)	0.0024 (13)	0.0025 (14)
C11	0.0162 (15)	0.0232 (16)	0.0187 (15)	0.0003 (11)	0.0008 (11)	−0.0018 (12)
C12	0.0237 (17)	0.0238 (17)	0.0255 (18)	−0.0004 (13)	0.0028 (13)	0.0033 (13)
C13	0.0210 (16)	0.033 (2)	0.0252 (16)	0.0056 (15)	−0.0003 (12)	0.0026 (15)
C14	0.0188 (16)	0.0252 (16)	0.0162 (14)	−0.0013 (12)	0.0023 (12)	−0.0001 (12)

Geometric parameters (Å, º)

Na1—O1^{i}	2.342 (3)	O5—C8	1.391 (5)
Na1—O2^{ii}	2.434 (3)	C1—C2	1.511 (5)
Na1—O4^{iii}	2.494 (3)	C2—C7	1.382 (5)
Na1—O2	2.517 (3)	C2—C3	1.394 (5)
Na1—O3^{iii}	2.789 (3)	C3—C4	1.399 (5)
Na2—O3^{iv}	2.285 (3)	C3—H3	0.9300
Na2—O4^{iii}	2.326 (3)	C4—C5	1.388 (5)
Na2—O2	2.435 (3)	C4—H4	0.9300
Na2—O4^{v}	2.453 (3)	C5—C6	1.389 (6)
O1—C1	1.252 (5)	C6—C7	1.404 (5)
O1—Na1^{vi}	2.342 (3)	C6—H6	0.9300
O1—Na3^{vi}	2.784 (4)	C7—H7	0.9300
O2—C1	1.268 (4)	C8—C9	1.382 (6)
O2—Na1^{vii}	2.434 (3)	C8—C13	1.384 (6)
O3—C14	1.260 (5)	C9—C10	1.389 (5)
O3—Na2^{viii}	2.285 (3)	C9—H9	0.9300
O3—Na3^{ix}	2.774 (4)	C10—C11	1.394 (5)
O3—Na1^{x}	2.789 (3)	C10—H10	0.9300
O4—C14	1.266 (5)	C11—C12	1.393 (5)
O4—Na2^{x}	2.326 (3)	C11—C14	1.509 (5)
O4—Na2^{xi}	2.453 (3)	C12—C13	1.401 (5)
O4—Na1^{x}	2.494 (3)	C12—H12	0.9300
O5—C5	1.381 (4)	C13—H13	0.9300
O1^{i}—Na1—O2^{ii}	128.52 (12)	O2—C1—C2	117.6 (3)
O1^{i}—Na1—O4^{iii}	96.84 (11)	C7—C2—C3	119.4 (3)
O2^{ii}—Na1—O4^{iii}	123.07 (11)	C7—C2—C1	121.1 (3)
O1^{i}—Na1—O2	84.62 (11)	C3—C2—C1	119.5 (3)
O2^{ii}—Na1—O2	124.75 (10)	C2—C3—C4	120.5 (3)
O4^{iii}—Na1—O2	86.69 (10)	C2—C3—H3	119.7
O1^{i}—Na1—O3^{iii}	144.60 (11)	C4—C3—H3	119.7
O2^{ii}—Na1—O3^{iii}	76.17 (10)	C5—C4—C3	119.1 (3)
O4^{iii}—Na1—O3^{iii}	49.58 (9)	C5—C4—H4	120.4
O2—Na1—O3^{iii}	101.66 (10)	C3—C4—H4	120.4
O3^{iv}—Na2—O4^{iii}	101.63 (12)	O5—C5—C4	115.2 (3)
O3^{iv}—Na2—O2	86.45 (11)	O5—C5—C6	123.4 (3)
O4^{iii}—Na2—O2	92.48 (11)	C4—C5—C6	121.3 (3)
O3^{iv}—Na2—O4^{v}	101.41 (12)	C5—C6—C7	118.6 (3)
O4^{iii}—Na2—O4^{v}	135.10 (11)	C5—C6—H6	120.7
O2—Na2—O4^{v}	126.93 (11)	C7—C6—H6	120.7
O2—Na2—Na3^{vi}	72.45 (9)	C2—C7—C6	121.0 (3)
C1—O1—Na1^{vi}	140.4 (3)	C2—C7—H7	119.5
C1—O1—Na3^{vi}	102.7 (2)	C6—C7—H7	119.5
Na1^{vi}—O1—Na3^{vi}	92.50 (11)	C9—C8—C13	121.6 (3)
C1—O2—Na1^{vii}	115.6 (2)	C9—C8—O5	118.7 (4)
C1—O2—Na2	106.9 (2)	C13—C8—O5	119.4 (4)

Na1^{vii}—O2—Na2	101.34 (11)	C8—C9—C10	119.6 (3)
C1—O2—Na1	120.0 (2)	C8—C9—H9	120.2
Na1^{vii}—O2—Na1	117.45 (12)	C10—C9—H9	120.2
Na2—O2—Na1	88.21 (10)	C9—C10—C11	120.2 (4)
C14—O3—Na2^{viii}	154.6 (3)	C9—C10—H10	119.9
C14—O3—Na3^{ix}	128.3 (2)	C11—C10—H10	119.9
Na2^{viii}—O3—Na3^{ix}	73.42 (10)	C12—C11—C10	119.4 (3)
C14—O3—Na1^{x}	83.5 (2)	C12—C11—C14	120.1 (3)
Na2^{viii}—O3—Na1^{x}	95.35 (10)	C10—C11—C14	120.4 (3)
Na3^{ix}—O3—Na1^{x}	68.61 (9)	C11—C12—C13	120.6 (3)
C14—O4—Na2^{x}	129.7 (2)	C11—C12—H12	119.7
C14—O4—Na2^{xi}	115.0 (2)	C13—C12—H12	119.7
Na2^{x}—O4—Na2^{xi}	115.15 (12)	C8—C13—C12	118.6 (4)
C14—O4—Na1^{x}	96.8 (2)	C8—C13—H13	120.7
Na2^{x}—O4—Na1^{x}	91.23 (10)	C12—C13—H13	120.7
Na2^{xi}—O4—Na1^{x}	84.93 (10)	O3—C14—O4	124.1 (3)
C5—O5—C8	120.4 (3)	O3—C14—C11	118.2 (3)
O1—C1—O2	123.7 (3)	O4—C14—C11	117.7 (3)
O1—C1—C2	118.7 (3)		

O3^{iv}—Na2—O2—C1	−128.5 (2)	C3—C4—C5—O5	−174.1 (4)
O4^{iii}—Na2—O2—C1	130.0 (2)	C3—C4—C5—C6	1.9 (6)
O4^{v}—Na2—O2—C1	−26.9 (3)	O5—C5—C6—C7	173.5 (3)
O3^{iv}—Na2—O2—Na1^{vii}	−7.05 (12)	C4—C5—C6—C7	−2.2 (6)
O4^{iii}—Na2—O2—Na1^{vii}	−108.56 (12)	C3—C2—C7—C6	0.7 (6)
O4^{v}—Na2—O2—Na1^{vii}	94.58 (14)	C1—C2—C7—C6	−178.9 (3)
O3^{iv}—Na2—O2—Na1	110.60 (11)	C5—C6—C7—C2	0.9 (6)
O4^{iii}—Na2—O2—Na1	9.09 (11)	C5—O5—C8—C9	90.4 (5)
O4^{v}—Na2—O2—Na1	−147.78 (12)	C5—O5—C8—C13	−96.2 (5)
O1^{i}—Na1—O2—C1	−19.8 (3)	C13—C8—C9—C10	−1.9 (6)
O2^{ii}—Na1—O2—C1	114.3 (2)	O5—C8—C9—C10	171.3 (3)
O4^{iii}—Na1—O2—C1	−117.0 (3)	C8—C9—C10—C11	1.3 (6)
O3^{iii}—Na1—O2—C1	−164.5 (3)	C9—C10—C11—C12	0.7 (5)
C14^{iii}—Na1—O2—C1	−138.8 (3)	C9—C10—C11—C14	−179.5 (3)
O1^{i}—Na1—O2—Na1^{vii}	−169.42 (13)	C10—C11—C12—C13	−2.2 (5)
O2^{ii}—Na1—O2—Na1^{vii}	−35.3 (2)	C14—C11—C12—C13	178.0 (3)
O4^{iii}—Na1—O2—Na1^{vii}	93.37 (13)	C9—C8—C13—C12	0.5 (6)
O3^{iii}—Na1—O2—Na1^{vii}	45.83 (14)	O5—C8—C13—C12	−172.7 (3)
C14^{iii}—Na1—O2—Na1^{vii}	71.53 (14)	C11—C12—C13—C8	1.6 (6)
O1^{i}—Na1—O2—Na2	88.72 (11)	Na2^{viii}—O3—C14—O4	113.0 (6)
O2^{ii}—Na1—O2—Na2	−137.17 (13)	Na3^{ix}—O3—C14—O4	−31.9 (5)
O4^{iii}—Na1—O2—Na2	−8.48 (10)	Na1^{x}—O3—C14—O4	24.2 (3)
O3^{iii}—Na1—O2—Na2	−56.02 (11)	Na2^{viii}—O3—C14—C11	−66.2 (7)
Na1^{vi}—O1—C1—O2	−69.3 (5)	Na3^{ix}—O3—C14—C11	148.8 (3)
Na3^{vi}—O1—C1—O2	40.8 (4)	Na1^{x}—O3—C14—C11	−155.1 (3)
Na1^{vi}—O1—C1—C2	111.7 (4)	Na2^{viii}—O3—C14—Na1^{x}	88.8 (6)
Na3^{vi}—O1—C1—C2	−138.3 (3)	Na3^{ix}—O3—C14—Na1^{x}	−56.1 (2)
Na1^{vii}—O2—C1—O1	−88.5 (4)	Na2^{x}—O4—C14—O3	70.0 (5)

Na2—O2—C1—O1	23.4 (4)	Na2^{xi}—O4—C14—O3	−114.9 (4)
Na1—O2—C1—O1	121.4 (3)	Na1^{x}—O4—C14—O3	−27.3 (4)
Na1^{vii}—O2—C1—C2	90.6 (3)	Na2^{x}—O4—C14—C11	−110.7 (3)
Na2—O2—C1—C2	−157.5 (2)	Na2^{xi}—O4—C14—C11	64.4 (3)
Na1—O2—C1—C2	−59.6 (4)	Na1^{x}—O4—C14—C11	152.0 (3)
O1—C1—C2—C7	−8.4 (5)	Na2^{x}—O4—C14—Na1^{x}	97.3 (3)
O2—C1—C2—C7	172.5 (3)	Na2^{xi}—O4—C14—Na1^{x}	−87.57 (17)
O1—C1—C2—C3	172.0 (4)	C12—C11—C14—O3	11.6 (5)
O2—C1—C2—C3	−7.1 (5)	C10—C11—C14—O3	−168.2 (3)
C7—C2—C3—C4	−1.0 (5)	C12—C11—C14—O4	−167.7 (3)
C1—C2—C3—C4	178.6 (3)	C10—C11—C14—O4	12.5 (5)
C2—C3—C4—C5	−0.3 (6)	C12—C11—C14—Na1^{x}	−95.3 (6)
C8—O5—C5—C4	−146.1 (4)	C10—C11—C14—Na1^{x}	84.9 (6)
C8—O5—C5—C6	37.9 (6)		

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