# metal-organic compounds

# Poly[[hexa-*μ*-aqua-diaquabis(*μ*₄-dihydrogen benzene-1,2,4,5-tetra-carboxylato)magnesiumdisodium] dihydrate]

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The asymmetric unit of the title compound, $\{[MgNa_2(C_{10}H_4O_8)_2(H_2O)_8]\cdot 2H_2O\}_n$, contains one octahedrally coordinated $Mg^{II}$ atom (site symmetry 2/*m*), one octahedrally coordinated $Na^{I}$ atom (site symmetry 2) and one half of the dihydrogen benzene-1,2,4,5-tetracarboxylate (btec) ligand, the second half of the ligand being generated by a twofold rotation axis. The basic framework of the title compound features infinite (–Na–Na–Mg–)$_n$ chains along $[10\bar{1}]$ with the metal cations bridged by the coordinating water molecules. The chains are isolated from each other by $\mu_4$-bridging btec ligands, which form intermolecular O—H···O hydrogen bonds to uncoordinated water molecules and the coordinated water molecules of a neighbouring chain. In each btec ligand, there are also intramolecular O—H···O hydrogen bonds.

## Related literature

For structures based on the H₄btec ligand, see: Gong & Zhang (2011); Liu *et al.* (2009, 2010); Zhang *et al.* (2007).
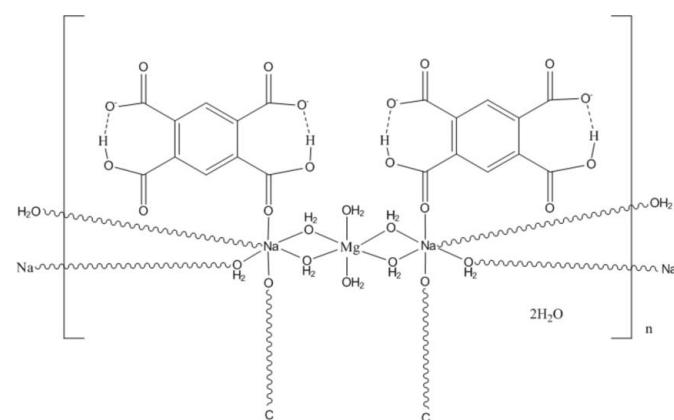


## Experimental

### Crystal data

| | |
|---|---|
| $[MgNa_2(C_{10}H_4O_8)_2(H_2O)_8]\cdot 2H_2O$ | $V = 1502.3$ (5) Å³ |
| $M_r = 754.71$ | $Z = 2$ |
| Monoclinic, $C2/m$ | Mo $K\alpha$ radiation |
| $a = 7.3335$ (13) Å | $\mu = 0.20$ mm⁻¹ |
| $b = 20.155$ (4) Å | $T = 296$ K |
| $c = 10.4450$ (18) Å | $0.20 \times 0.05 \times 0.05$ mm |
| $\beta = 103.325$ (3)° | |

### Data collection

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 4088 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | 1440 independent reflections |
| | 1272 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.961$, $T_{max} = 0.990$ | $R_{int} = 0.022$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.030$ | 122 parameters |
| $wR(F^2) = 0.089$ | H-atom parameters constrained |
| $S = 1.08$ | $\Delta\rho_{max} = 0.23$ e Å⁻³ |
| 1440 reflections | $\Delta\rho_{min} = -0.21$ e Å⁻³ |

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3···O2 | 1.06 | 1.35 | 2.3827 (17) | 163 |
| O5—H5···O7 | 0.90 | 1.83 | 2.7313 (14) | 173 |
| O6—H6···O4$^{i}$ | 0.90 | 1.97 | 2.8519 (15) | 167 |
| O7—H7···O2$^{ii}$ | 0.86 | 1.91 | 2.7699 (14) | 173 |
| O8—H8···O3$^{iii}$ | 0.85 | 1.94 | 2.7779 (14) | 172 |
| O9—H9···O4$^{ii}$ | 0.85 | 1.91 | 2.7559 (14) | 171 |

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2296).

## References

Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
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Zhang, D. J., Song, T. Y., Zhang, P., Shi, J., Wang, Y., Wang, L., Ma, K. R., Yin, W. R., Zhao, J., Fan, Y. & Xu, J. N. (2007). *Inorg. Chem. Commun.* **10**, 876–879.

# supporting information

# Poly[[hexa-*μ*-aqua-diaquabis(*μ*₄-dihydrogen benzene-1,2,4,5-tetracarboxylato)magnesiumdisodium] dihydrate]

**Dan Zhao, Peng Liang, Yan-Feng Li, Sen Qiu and Jun-Ran Ren**

### S1. Comment

In recent years, much attention has been paid to coordination polymer materials based on covalent interactions or supramolecular contacts, and huge numbers of novel compounds with interesting structures and topologies have been reported. As part of this research benzene-1,2,4,5-tetracarboxylate (btec) can be used as a ligand to form various supramolecular architectures with its four rigid carboxyl groups (Gong *et al.*, 2011; Liu *et al.*, 2009; Liu *et al.*, 2010; Zhang *et al.*, 2007). In order to enrich this family of compounds, we used the hydrothermal method to synthesise the title compound, a new sodium(I)-magnesium(II) complex, that is, $Na_2Mg(btec)_2(H_2O)_8.2(H_2O)$, where btec = benzene-1,2,4,5-tetracarboxylate, and we determined its structure by single-crystal X-ray diffraction.

As shown in Fig. 1, the asymmetric unit of the title compound contains one octahedrally coordinated magnesium atom, one octahedrally coordinated sodium atom and half a benzene-1,2,4,5-tetracarboxylate (btec) ligand. Each btec ligands contains two intramolecular O–H···O hydrogen bonds, with the H atoms bonded to atoms O3 and O2, and connects two Na atoms in a $μ_2$– manner. Each Na atom is coordinated by two *cis* carboxylate oxygen atoms from two btec ligands and by four water molecules, while each Mg is coordinated by six water molecules. The Na–O bond distances range from 2.2669 (12) to 2.6146 (18) Å, while the Mg–O bond lengths are slightly longer ranging from 2.0301 (14) to 2.1008 (14) Å. Furthermore, $NaO_6$ octahedra and $MgO_6$ octahedra are connected *via* coordinated water molecules to form a one-dimensional infinite $(–Na–Na–Mg–)_n$ chain, as shown in Fig. 2. O—H···O hydrogen bonds link the coordinated and uncoordinated water molecules to neighbouring btec ligands (Table 1).

### S2. Experimental

A mixture of 1,2,4,5-benzene-tetracarboxylic (0.2 g), Na2CO3 (0.1 g), MgO(0.05 g) and $H_2O$ (15 ml) was heated at 448 K for 7 d in a sealed 25 ml Teflon-lined stainless steel vessel under autogenous pressure. After cooling to room temperature at a rate of 5 C h⁻¹, colourless prismatic crystals were obtained in low yield.

### S3. Refinement

The H atoms of C atoms were positioned geometrically and refined with a riding model, with C—H = 0.93 Å and $U_{iso}(H)$ = $1.2U_{eq}(C)$. The water H atoms were located in difference Fourier maps, and then refined with a riding model, with $U_{iso}(H)$ = $1.5U_{eq}(O)$.
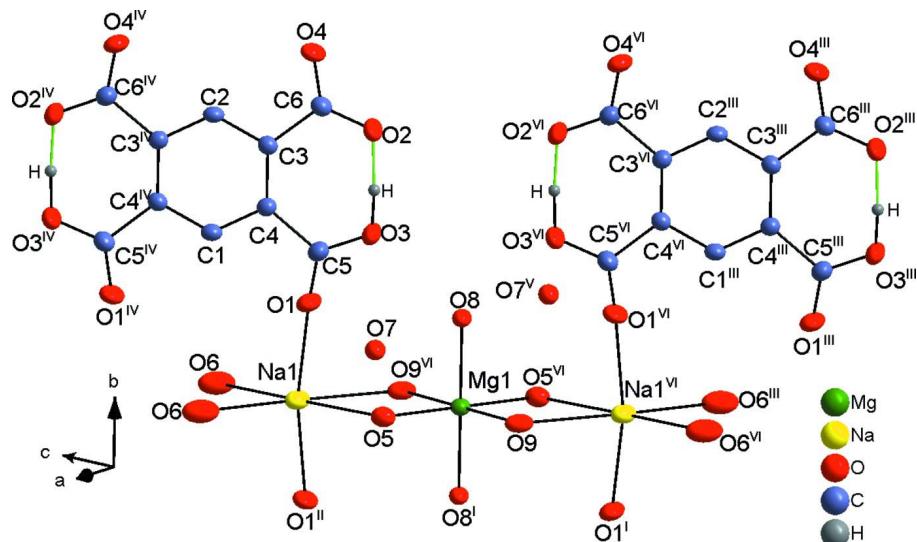
**Figure 1**

A view of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and hydrogen atoms are omitted for clarity, except for intramolecular hydrogen bonding H atoms in the btec ligands (indicated as pea green lines). [Symmetry codes: (i) -x, -y, -z; (ii) x, -y, z; (iii) x - 1, y, z - 1; (iv) -x + 1, y, -z + 1; (v) x - 1, y, z; (vi) -x, y, -z].
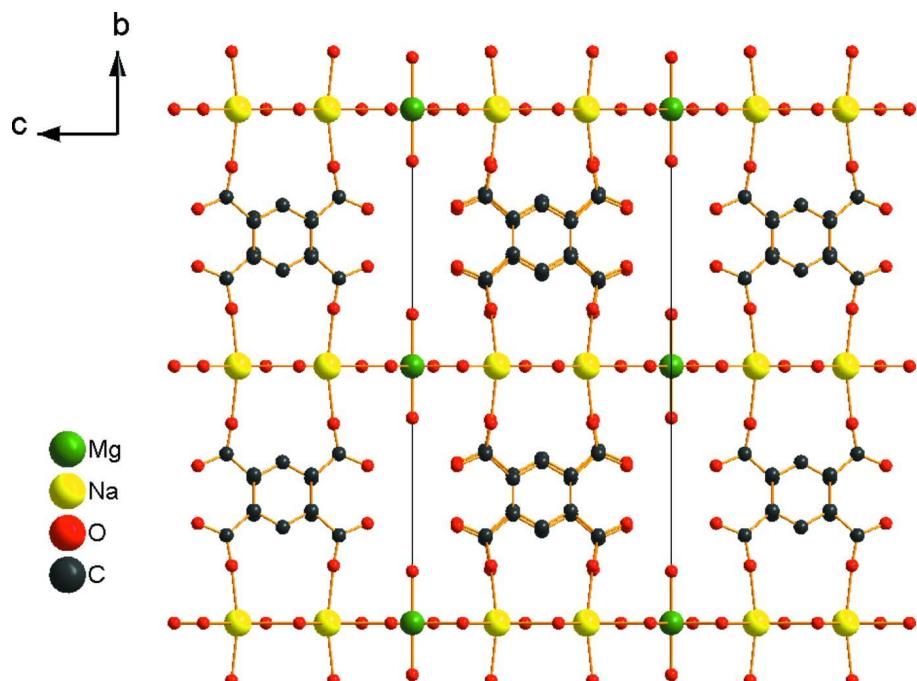


**Figure 2**

View of the crystal structure of the title compound along the a-axis.

**Poly[[hexa-*μ*-aqua-diaquabis(*μ*₄-dihydrogen benzene-1,2,4,5-tetracarboxylato)magnesium(II)disodium] dihydrate]**

*Crystal data*
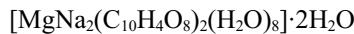
| | |
|---|---|
| $[MgNa_2(C_{10}H_4O_8)_2(H_2O)_8]\cdot2H_2O$ | $F(000) = 780$ |
| $M_r = 754.71$ | $D_x = 1.668$ Mg m$^{-3}$ |
| Monoclinic, $C2/m$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -C 2y | Cell parameters from 2031 reflections |
| $a = 7.3335$ (13) Å | $\theta = 2.9–27.8°$ |
| $b = 20.155$ (4) Å | $\mu = 0.20$ mm$^{-1}$ |
| $c = 10.4450$ (18) Å | $T = 296$ K |
| $\beta = 103.325$ (3)° | Prism, colourless |
| $V = 1502.3$ (5) Å$^3$ | $0.20 \times 0.05 \times 0.05$ mm |
| $Z = 2$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 4088 measured reflections |
| Radiation source: fine-focus sealed tube | 1440 independent reflections |
| Graphite monochromator | 1272 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 83.33 pixels mm$^{-1}$ | $R_{int} = 0.022$ |
| $\omega$ scans | $\theta_{max} = 25.5°$, $\theta_{min} = 2.0°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -8\rightarrow8$ |
| | $k = -24\rightarrow22$ |
| $T_{min} = 0.961$, $T_{max} = 0.990$ | $l = -11\rightarrow12$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.030$ | H-atom parameters constrained |
| $wR(F^2) = 0.089$ | $w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 0.7471P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.08$ | |
| 1440 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 122 parameters | $\Delta\rho_{max} = 0.23$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.21$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc$^*$=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$ |
| Secondary atom site location: difference Fourier map | Extinction coefficient: 0.0033 (7) |

*Special details*

**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)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| Mg1 | 0.0000 | 0.0000 | 0.0000 | 0.0220 (2) |

| | | | |
|---|---|---|---|
| Na1 | 0.31699 (13) | 0.0000 | 0.32732 (8) | 0.0356 (3) |
| O1 | 0.30603 (18) | 0.11183 (5) | 0.30357 (11) | 0.0464 (3) |
| C1 | 0.5000 | 0.18685 (9) | 0.5000 | 0.0233 (4) |
| H1 | 0.5000 | 0.1407 | 0.5000 | 0.028* |
| O2 | 0.20225 (19) | 0.31210 (6) | 0.17351 (10) | 0.0487 (4) |
| C2 | 0.5000 | 0.32051 (9) | 0.5000 | 0.0221 (4) |
| H2 | 0.5000 | 0.3667 | 0.5000 | 0.027* |
| O3 | 0.20002 (18) | 0.19389 (6) | 0.17286 (10) | 0.0481 (4) |
| H3 | 0.2132 | 0.2456 | 0.1607 | 0.072* |
| C3 | 0.39709 (18) | 0.28869 (6) | 0.38857 (12) | 0.0211 (3) |
| O4 | 0.31030 (15) | 0.39579 (5) | 0.30165 (10) | 0.0339 (3) |
| C4 | 0.39692 (18) | 0.21864 (6) | 0.38884 (12) | 0.0214 (3) |
| O5 | 0.28991 (19) | 0.0000 | 0.08188 (14) | 0.0288 (3) |
| H5 | 0.3530 | 0.0340 | 0.0564 | 0.043* |
| C5 | 0.2960 (2) | 0.17086 (7) | 0.28270 (14) | 0.0283 (3) |
| O6 | 0.3317 (3) | 0.0000 | 0.56419 (17) | 0.0483 (5) |
| H6 | 0.2884 | −0.0368 | 0.5963 | 0.073* |
| C6 | 0.29702 (19) | 0.33570 (7) | 0.28103 (13) | 0.0258 (3) |
| O7 | 0.5000 | 0.09605 (7) | 0.0000 | 0.0311 (3) |
| H7 | 0.4367 | 0.1223 | −0.0590 | 0.047* |
| O8 | 0.0000 | 0.10073 (7) | 0.0000 | 0.0322 (4) |
| H8 | −0.0681 | 0.1262 | −0.0560 | 0.048* |
| O9 | 0.0320 (2) | 0.0000 | −0.19461 (14) | 0.0314 (4) |
| H9 | 0.0897 | 0.0325 | −0.2191 | 0.047* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mg1 | 0.0265 (5) | 0.0161 (4) | 0.0222 (5) | 0.000 | 0.0032 (4) | 0.000 |
| Na1 | 0.0521 (6) | 0.0188 (4) | 0.0328 (5) | 0.000 | 0.0034 (4) | 0.000 |
| O1 | 0.0678 (8) | 0.0176 (6) | 0.0428 (7) | −0.0038 (5) | −0.0098 (6) | −0.0044 (5) |
| C1 | 0.0259 (10) | 0.0152 (9) | 0.0275 (10) | 0.000 | 0.0037 (8) | 0.000 |
| O2 | 0.0697 (8) | 0.0256 (6) | 0.0343 (6) | 0.0023 (5) | −0.0222 (6) | 0.0038 (5) |
| C2 | 0.0262 (9) | 0.0136 (9) | 0.0258 (10) | 0.000 | 0.0046 (8) | 0.000 |
| O3 | 0.0683 (8) | 0.0244 (6) | 0.0350 (6) | −0.0028 (5) | −0.0224 (6) | −0.0032 (5) |
| C3 | 0.0216 (7) | 0.0186 (7) | 0.0225 (7) | 0.0007 (5) | 0.0038 (5) | 0.0014 (5) |
| O4 | 0.0478 (7) | 0.0177 (5) | 0.0335 (6) | 0.0032 (4) | 0.0040 (5) | 0.0050 (4) |
| C4 | 0.0215 (6) | 0.0185 (7) | 0.0231 (7) | −0.0010 (5) | 0.0031 (5) | −0.0012 (5) |
| O5 | 0.0280 (7) | 0.0221 (7) | 0.0363 (8) | 0.000 | 0.0070 (6) | 0.000 |
| C5 | 0.0318 (8) | 0.0214 (7) | 0.0282 (7) | −0.0012 (6) | 0.0000 (6) | −0.0036 (6) |
| O6 | 0.0713 (12) | 0.0291 (8) | 0.0533 (11) | 0.000 | 0.0321 (9) | 0.000 |
| C6 | 0.0282 (7) | 0.0211 (7) | 0.0263 (7) | 0.0011 (5) | 0.0028 (6) | 0.0028 (6) |
| O7 | 0.0357 (8) | 0.0214 (7) | 0.0304 (8) | 0.000 | −0.0046 (6) | 0.000 |
| O8 | 0.0419 (9) | 0.0162 (7) | 0.0299 (8) | 0.000 | −0.0094 (6) | 0.000 |
| O9 | 0.0469 (9) | 0.0185 (7) | 0.0324 (8) | 0.000 | 0.0166 (7) | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Mg1—O8 | 2.0301 (14) | O2—C6 | 1.2691 (17) |
| Mg1—O8<sup>i</sup> | 2.0302 (14) | O2—H3 | 1.3505 |
| Mg1—O9 | 2.0992 (14) | C2—C3 | 1.3895 (15) |
| Mg1—O9<sup>i</sup> | 2.0992 (14) | C2—C3<sup>iv</sup> | 1.3895 (15) |
| Mg1—O5<sup>i</sup> | 2.1008 (14) | C2—H2 | 0.9300 |
| Mg1—O5 | 2.1008 (14) | O3—C5 | 1.2865 (17) |
| Mg1—Na1<sup>i</sup> | 3.6645 (10) | O3—H3 | 1.0579 |
| Mg1—Na1 | 3.6646 (10) | C3—C4 | 1.4119 (18) |
| Na1—O1 | 2.2669 (12) | C3—C6 | 1.5225 (18) |
| Na1—O1<sup>ii</sup> | 2.2669 (12) | O4—C6 | 1.2301 (17) |
| Na1—O6 | 2.4515 (19) | C4—C5 | 1.5250 (18) |
| Na1—O5 | 2.5252 (16) | O5—H5 | 0.9007 |
| Na1—O6<sup>iii</sup> | 2.564 (2) | O6—Na1<sup>iii</sup> | 2.564 (2) |
| Na1—O9<sup>i</sup> | 2.6146 (18) | O6—H6 | 0.9011 |
| Na1—Na1<sup>iii</sup> | 3.9692 (17) | O7—H7 | 0.8628 |
| O1—C5 | 1.2088 (18) | O8—H8 | 0.8481 |
| C1—C4 | 1.3876 (15) | O9—Na1<sup>i</sup> | 2.6146 (17) |
| C1—C4<sup>iv</sup> | 1.3876 (15) | O9—H9 | 0.8510 |
| C1—H1 | 0.9300 | | |
| | | | |
| O8—Mg1—O8<sup>i</sup> | 180.0 | O1<sup>ii</sup>—Na1—Mg1 | 84.21 (4) |
| O8—Mg1—O9 | 90.0 | O6—Na1—Mg1 | 144.34 (6) |
| O8<sup>i</sup>—Mg1—O9 | 90.0 | O5—Na1—Mg1 | 33.73 (3) |
| O8—Mg1—O9<sup>i</sup> | 90.0 | O6<sup>iii</sup>—Na1—Mg1 | 140.26 (5) |
| O8<sup>i</sup>—Mg1—O9<sup>i</sup> | 90.0 | O9<sup>i</sup>—Na1—Mg1 | 34.15 (3) |
| O9—Mg1—O9<sup>i</sup> | 180.00 (8) | O1—Na1—Na1<sup>iii</sup> | 95.68 (4) |
| O8—Mg1—O5<sup>i</sup> | 90.0 | O1<sup>ii</sup>—Na1—Na1<sup>iii</sup> | 95.68 (4) |
| O8<sup>i</sup>—Mg1—O5<sup>i</sup> | 90.0 | O6—Na1—Na1<sup>iii</sup> | 38.69 (5) |
| O9—Mg1—O5<sup>i</sup> | 86.23 (6) | O5—Na1—Na1<sup>iii</sup> | 143.24 (5) |
| O9<sup>i</sup>—Mg1—O5<sup>i</sup> | 93.77 (6) | O6<sup>iii</sup>—Na1—Na1<sup>iii</sup> | 36.70 (4) |
| O8—Mg1—O5 | 90.0 | O9<sup>i</sup>—Na1—Na1<sup>iii</sup> | 148.88 (5) |
| O8<sup>i</sup>—Mg1—O5 | 90.0 | Mg1—Na1—Na1<sup>iii</sup> | 176.97 (4) |
| O9—Mg1—O5 | 93.77 (6) | C5—O1—Na1 | 175.97 (11) |
| O9<sup>i</sup>—Mg1—O5 | 86.23 (6) | C4—C1—C4<sup>iv</sup> | 125.01 (18) |
| O5<sup>i</sup>—Mg1—O5 | 180.0 | C4—C1—H1 | 117.5 |
| O8—Mg1—Na1<sup>i</sup> | 90.0 | C4<sup>iv</sup>—C1—H1 | 117.5 |
| O8<sup>i</sup>—Mg1—Na1<sup>i</sup> | 90.0 | C6—O2—H3 | 115.2 |
| O9—Mg1—Na1<sup>i</sup> | 44.36 (4) | C3—C2—C3<sup>iv</sup> | 125.01 (17) |
| O9<sup>i</sup>—Mg1—Na1<sup>i</sup> | 135.64 (4) | C3—C2—H2 | 117.5 |
| O5<sup>i</sup>—Mg1—Na1<sup>i</sup> | 41.87 (4) | C3<sup>iv</sup>—C2—H2 | 117.5 |
| O5—Mg1—Na1<sup>i</sup> | 138.13 (4) | C5—O3—H3 | 114.6 |
| O8—Mg1—Na1 | 90.0 | C2—C3—C4 | 117.42 (12) |
| O8<sup>i</sup>—Mg1—Na1 | 90.0 | C2—C3—C6 | 114.02 (12) |
| O9—Mg1—Na1 | 135.64 (4) | C4—C3—C6 | 128.56 (11) |
| O9<sup>i</sup>—Mg1—Na1 | 44.36 (4) | C1—C4—C3 | 117.57 (12) |
| O5<sup>i</sup>—Mg1—Na1 | 138.13 (4) | C1—C4—C5 | 113.34 (13) |

| | | | |
|---|---|---|---|
| O5—Mg1—Na1 | 41.87 (4) | C3—C4—C5 | 129.09 (11) |
| Na1$^i$—Mg1—Na1 | 180.0 | Mg1—O5—Na1 | 104.40 (6) |
| O1—Na1—O1$^{ii}$ | 167.72 (7) | Mg1—O5—H5 | 114.8 |
| O1—Na1—O6 | 95.89 (4) | Na1—O5—H5 | 112.0 |
| O1$^{ii}$—Na1—O6 | 95.89 (4) | O1—C5—O3 | 120.93 (13) |
| O1—Na1—O5 | 84.05 (4) | O1—C5—C4 | 119.43 (13) |
| O1$^{ii}$—Na1—O5 | 84.05 (4) | O3—C5—C4 | 119.64 (12) |
| O6—Na1—O5 | 178.07 (7) | Na1—O6—Na1$^{iii}$ | 104.61 (6) |
| O1—Na1—O6$^{iii}$ | 93.16 (4) | Na1—O6—H6 | 116.0 |
| O1$^{ii}$—Na1—O6$^{iii}$ | 93.16 (4) | Na1$^{iii}$—O6—H6 | 103.9 |
| O6—Na1—O6$^{iii}$ | 75.39 (6) | O4—C6—O2 | 121.94 (13) |
| O5—Na1—O6$^{iii}$ | 106.54 (6) | O4—C6—C3 | 118.58 (12) |
| O1—Na1—O9$^i$ | 86.35 (4) | O2—C6—C3 | 119.48 (12) |
| O1$^{ii}$—Na1—O9$^i$ | 86.35 (4) | Mg1—O8—H8 | 127.2 |
| O6—Na1—O9$^i$ | 110.19 (6) | Mg1—O9—Na1$^i$ | 101.49 (6) |
| O5—Na1—O9$^i$ | 67.88 (5) | Mg1—O9—H9 | 117.8 |
| O6$^{iii}$—Na1—O9$^i$ | 174.41 (6) | Na1$^i$—O9—H9 | 109.5 |
| O1—Na1—Mg1 | 84.21 (4) | | |

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) *x*, −*y*, *z*; (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*+1, *y*, −*z*+1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3···O2 | 1.06 | 1.35 | 2.3827 (17) | 163 |
| O5—H5···O7 | 0.90 | 1.83 | 2.7313 (14) | 173 |
| O6—H6···O4$^v$ | 0.90 | 1.97 | 2.8519 (15) | 167 |
| O7—H7···O2$^{vi}$ | 0.86 | 1.91 | 2.7699 (14) | 173 |
| O8—H8···O3$^{vii}$ | 0.85 | 1.94 | 2.7779 (14) | 172 |
| O9—H9···O4$^{vi}$ | 0.85 | 1.91 | 2.7559 (14) | 171 |

Symmetry codes: (v) −*x*+1/2, *y*−1/2, −*z*+1; (vi) −*x*+1/2, −*y*+1/2, −*z*; (vii) −*x*, *y*, −*z*.