Poly[μ₃-aqua-aqua-μ₅-(4-nitrobenzoato)-caesium]

Graham Smith

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Poly[mu3-aqua-aqua-mu5-(4-nitrobenzoato)-caesium]

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Key indicators: single-crystal X-ray study; T = 200 K; mean r(C–C) = 0.006 Å; R factor = 0.032; wR factor = 0.074; data-to-parameter ratio = 15.1.

In the structure of the title complex, [Cs(C7H4NO2)(H2O)2]2n, the caesium salt of 4-nitrobenzoic acid, the irregular CsO9 coordination sphere comprises three bridging nitro O-atom donors, a bidentate carboxylate O,O'-chelate interaction, a triple-bridging water molecule and a monodentate water molecule. A three-dimensional framework polymer is generated, within which there are water–carboxylate O—H⋯O and water–water O—H⋯O hydrogen-bonding interactions.

Related literature

For structures of alkali metal salts of 4-nitrobenzoic acid, see: Turowska-Tyrk et al. (1988) (Na); Srivastava & Speakman (1961) (K). For the structures of Na, K and Cs complexes with 4-nitroantranilic acid, see: Smith & Wermuth (2011); Smith (2013). For the structures of the 4-nitrobenzoic acid polymorphs, see: Groth (1980); Tonogaki et al. (1993); Bolte (2009).

Experimental

Crystal data

\[\text{Cs(C7H4NO2)(H2O)2}\]

\(M_r = 335.05\)

Monoclinic, \(P2_1/n\)

\(a = 6.0700 (3)\) Å

\(b = 7.1073 (4)\) Å

\(c = 24.2183 (13)\) Å

\(\beta = 94.035 (5)\)°

\(V = 1042.22 (10)\) Å³

\(Z = 4\)

Mo Kα radiation

\(\mu = 3.56\) mm⁻¹

\(T = 200\) K

Data collection

Oxford Diffraction Gemini-S CCD-detector diffractometer

\(\bar{R} (I^{2} > 2\sigma(I)) = 0.032\)

\(wR (F^2) = 0.074\)

\(\bar{S} = 1.15\)

2057 reflections

6334 measured reflections

2057 independent reflections

1836 reflections with \(I > 2\sigma(I)\)

\(R_{int} = 0.036\)

Refinement

\(R(F^2) = 0.074\)

\(wR(F^2) = 0.074\)

\(S = 1.15\)

136 parameters

H-atom parameters constrained

\(\Delta P_{max} = 0.56\) e Å⁻³

\(\Delta P_{min} = -0.67\) e Å⁻³

Table 1

Selected bond lengths (Å).

\(\text{Cs1—O1W} \quad 3.126 (3) \quad \text{Cs1—O1}'' \quad 3.215 (3)\)

\(\text{Cs1—O2W} \quad 3.253 (3) \quad \text{Cs1—O12}'' \quad 3.338 (4)\)

\(\text{Cs1—O41} \quad 3.244 (4) \quad \text{Cs1—O2W}'' \quad 3.047 (4)\)

\(\text{Cs1—O42}'' \quad 3.248 (4) \quad \text{Cs1—O41}'' \quad 3.310 (4)\)

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

Table 2

Hydrogen-bond geometry (Å, °).

\(D—H···A\)

\(D—H\)

\(H···A\)

\(D···A\)

\(D—H···A\)

\(O1W—H1W···O12''\) 0.82 1.88 2.694 (5) 174

\(O1W—H2W···O11''\) 0.93 1.81 2.728 (4) 173

\(O2W—H21W···O1W''\) 0.79 1.99 2.749 (5) 162

\(O2W—H22W···O11''\) 0.84 1.91 2.753 (5) 174

Symmetry codes: (iv) \(-x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}\); (v) \(-x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}\); (vi) \(-x+1, -y, z+1\).

Data collection: Crystals PRO (Agilent, 2012); cell refinement: Crystals PRO; data reduction: Crystals PRO; program(s) used to solve structure: SIR92 (Altomare et al., 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); within WinGX (Farrugia, 2012); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: PLATON.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5666).

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supplementary materials

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Poly[$\mu_3$-aqua-aqua-$\mu_5$-(4-nitrobenzoato)-caesium]

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1. Comment

4-Nitrobenzoic acid (PNBA) has proved to be a useful ligand for the preparation of metal complexes, which are mainly monomeric but rarely involve the nitro group in coordination. With the known alkali metal salts of PNBA, the sodium salt (a trihydrate) (Turowska-Tyrk et al., 1988) and the potassium salt (a 1:1 salt–acid adduct) (Srivastava & Speakman, 1961), coordination polymeric structures are formed, but the structures of the rubidium and caesium salts have not been reported. The reaction of 4-nitrobenzoic acid with caesium hydroxide in aqueous ethanol afforded good crystals of the title Cs complex, [Cs(C$_7$H$_4$NO$_2$)(H$_2$O)$_2$]$_n$, and the structure is reported herein.

In this structure (Fig. 1), the irregular CsO$_9$ coordinate polyhedron comprises a bidentate carboxylate $O,O'$-chelate interaction, three O-donors from an $O,O'$-bridging nitro group, three O donors from a triple-bridging water molecule (O2W) and a monodentate water molecule (O1W) [Cs—O, 3.047 (4)–3.338 (4) Å] (Table 1). The bridging extensions in the two-dimensional sheet substructures which extend along the (0 0 1) plane include a centrosymmetric water–carboxyl quadruple cage (Fig. 2) (Cs···Cs$^{iii}$ = 4.2610 (6) Å) [for symmetry code (iii), see Table 2]. The $p$-related carboxyl and nitro substituent groups of the PNBA ligand link the sheets across $c$, and generate an overall a three-dimensional coordination polymer (Fig. 3). This type of structure extension through the $p$-related benzoate carboxyl and nitro functional groups is similar to that found in other alkali metal complexes with the 4-nitroanthranilate salts of sodium (a dihydrate) and potassium (a monohydrate) (Smith, 2013), and caesium (a monohydrate) (Smith & Wermuth, 2011).

The crystal structure of the title complex polymer is stabilized by intra-sheet water O—H···Ocarboxyl and O—H···Owater hydrogen-bonding interactions (Table 2). No inter-ring $\pi$—$\pi$ interactions are present [minimum ring centroid separation 4.643 (2) Å]. The PABA ligand in the complex is essentially planar [torsion angles C2—C1—C11—O12 = 177.9 (4)° (carboxyl) and C3—C4—N41—O41 = 177.5 (4)° (nitro)]. This conformation is similar to that found in both monoclinic polymorphs of the parent acid [Tonogaki et al., 1993; Groth, 1980; Bolte, 2009].

2. Experimental

The title compound was synthesized by heating together for 10 minutes, 0.5 mmol of 4-nitrobenzoic acid and 0.5 mmol of CsOH in 15 ml of 10% ethanol–water. Partial room temperature evaporation of the solution gave colourless elongated crystal plates of the title complex from which a specimen was cleaved for the X-ray analysis.

3. Refinement

Carbon-bound hydrogen atoms were placed in calculated positions [C—H = 0.95 Å] and allowed to ride in the refinement, with $U_{iso}(H) = 1.2 U_{eq}(C)$. Hydrogen atoms of the coordinated water molecule were located in a difference Fourier map but were subsequently allowed to ride, with $U_{iso}(H) = 1.5 U_{eq}(O)$. 

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Computing details

Data collection: CrysAlis PRO (Agilent, 2012); cell refinement: CrysAlis PRO (Agilent, 2012); data reduction: CrysAlis PRO (Agilent, 2012); program(s) used to solve structure: SIR92 (Altomare et al., 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008) within WinGX (Farrugia, 2012); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: PLATON (Spek, 2009).

Figure 1

The molecular configuration and atom-numbering scheme for the coordination polyhedron of title complex, with non-H atoms drawn as 40% probability displacement ellipsoids. For symmetry codes: see Table 1.

Figure 2

A partial expansion of the CsO$_9$ coordination sphere in the polymeric structure. For symmetry codes: (vii) $x + 1, y, z$; (viii) $-x, -y, -z + 1$. For other symmetry codes, see Fig. 1 and Table 1.
Figure 3
The packing of the structure in the unit cell viewed along a. Hydrogen-bonding associations are shown as dashed lines.

Poly[μ$_3$-aqua-aqua-μ$_5$-(4-nitrobenzoato)-caesium]

Crystal data

$[\text{Cs(C}_7\text{H}_4\text{NO}_2)(\text{H}_2\text{O})_2]$  $F(000) = 640$

$M_r = 335.05$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 6.0700$ (3) Å  $D_x = 2.135$ Mg m$^{-3}$

$b = 7.1073$ (4) Å  $\text{Mo } K\alpha$ radiation, $\lambda = 0.71073$ Å

$c = 24.2183$ (13) Å  $\theta = 3.5–28.1^\circ$

$\beta = 94.035$ (5)$^\circ$

$V = 1042.22$ (10) Å$^3$

$Z = 4$

$\mu = 3.56$ mm$^{-1}$

Cell parameters from 2366 reflections

$T = 200$ K

Plate, colourless

0.28 × 0.18 × 0.05 mm

Data collection

Oxford Diffraction Gemini-S CCD-detector

diffractometer

Radiation source: Enhance (Mo) X-ray source

Graphite monochromator

Detector resolution: 16.077 pixels mm$^{-1}$

$\omega$ scans

$R_{int} = 0.036$

$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 3.3^\circ$

$6334$ measured reflections

$\omega$ scans

482 independent reflections

$1836$ reflections with $I > 2\sigma(I)$

$2057$ independent reflections

$1836$ reflections with $I > 2\sigma(I)$

$\Delta \rho_{\text{max}} = 0.56$ e Å$^{-3}$

$\Delta \rho_{\text{min}} = -0.67$ e Å$^{-3}$

Refinement

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.074$

$S = 1.15$

2057 reflections

136 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

$w = 1/[\sigma^2(F^2) + (0.0285P)^2 + 0.878P]$

where $P = (F^2 + 2F_c^2)/3$

$(\Delta \sigma)_{\text{max}} = 0.001$

$\Delta \rho_{\text{max}} = 0.56$ e Å$^{-3}$

$\Delta \rho_{\text{min}} = -0.67$ e Å$^{-3}$
supplementary materials

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All esds are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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 (Å$^2$)

| Atom | x     | y     | z     | $U_{	ext{eq}}$ |
|------|-------|-------|-------|--------------|
| Cs1  | 0.25378(4) | 0.19824(4) | 0.47189(1) | 0.0259(1) |
| O1W  | 0.2785(5)  | 0.5049(5)  | 0.56462(14) | 0.0354(11) |
| O2W  | 0.7695(5)  | 0.2283(5)  | 0.51753(15) | 0.0347(11) |
| O11  | 0.3802(5)  | 0.0475(5)  | 0.10793(14) | 0.0333(11) |
| O12  | 0.0968(5)  | -0.0945(5) | 0.14338(15) | 0.0400(11) |
| O41  | 0.6184(7)  | -0.0192(5) | 0.40379(16) | 0.0467(14) |
| O42  | 0.9117(7)  | 0.0828(7)  | 0.36824(17) | 0.0576(16) |
| N41  | 0.7213(7)  | 0.0261(6)  | 0.36407(17) | 0.0311(12) |
| C1   | 0.4023(7)  | -0.0137(5) | 0.20429(19) | 0.0189(11) |
| C2   | 0.6135(7)  | 0.0617(6)  | 0.2120(2)   | 0.0236(14) |
| C3   | 0.7195(7)  | 0.0745(6)  | 0.26440(19) | 0.0235(14) |
| C4   | 0.6093(7)  | 0.0113(6)  | 0.30818(19) | 0.0229(14) |
| C5   | 0.4009(7)  | -0.0646(6) | 0.30250(19) | 0.0250(14) |
| C6   | 0.2985(7)  | -0.0777(6) | 0.25023(19) | 0.0223(14) |
| C11  | 0.2830(7)  | -0.0201(6) | 0.1477(2)   | 0.0252(14) |
| H2   | 0.68620    | 0.10490    | 0.18090     | 0.0280*    |
| H3   | 0.86400    | 0.12560    | 0.26980     | 0.0280*    |
| H5   | 0.32940    | -0.10700   | 0.33390     | 0.0300*    |
| H6   | 0.15490    | -0.13100   | 0.24530     | 0.0270*    |
| H11W | 0.37890    | 0.53710    | 0.58680     | 0.0530*    |
| H12W | 0.14960    | 0.48830    | 0.58230     | 0.0530*    |
| H21W | 0.72670    | 0.30190    | 0.49470     | 0.0520*    |
| H22W | 0.79800    | 0.29200    | 0.54650     | 0.0520*    |

Atomic displacement parameters (Å$^2$)

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|------|----------|----------|----------|----------|----------|----------|
| Cs1  | 0.0259(2) | 0.0272(2) | 0.0240(2) | 0.0000(1) | -0.0015(1) | 0.0013(1) |
| O1W  | 0.0348(18)| 0.052(2)  | 0.0189(19)| -0.0046(17)| -0.0014(14)| 0.0006(16)|
| O2W  | 0.044(2) | 0.0296(17)| 0.030(2)  | -0.0030(15)| -0.0003(16)| -0.0028(15)|
| O11  | 0.0334(18)| 0.049(2)  | 0.0173(19)| -0.0022(16)| 0.0010(14) | -0.0089(16)|
| O12  | 0.0335(19)| 0.055(2)  | 0.030(2)  | -0.0104(18)| -0.0092(15)| 0.0061(18)|
| O41  | 0.065(3) | 0.056(2)  | 0.018(2)  | 0.002(2)   | -0.0040(18)| 0.0036(18)|
| O42  | 0.049(2) | 0.085(3)  | 0.036(3)  | -0.015(2)  | -0.0171(19)| -0.007(2) |
| N41  | 0.042(2) | 0.033(2)  | 0.017(2)  | 0.0051(19) | -0.0076(19)| -0.0057(18)|
| C1   | 0.020(2) | 0.0163(19)| 0.020(2)  | 0.0015(17) | -0.0021(18)| 0.0017(18)|
| C2   | 0.027(2) | 0.021(2)  | 0.023(3)  | -0.0022(18)| 0.0028(19) | 0.0012(19)|
| C3   | 0.023(2) | 0.024(2)  | 0.023(3)  | -0.0029(19)| -0.0008(19)| -0.0037(19)|

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### Geometric parameters (Å, °)

| Bond/Distance | Value (Å) | Bond/Distance | Value (Å) |
|---------------|-----------|---------------|-----------|
| Cs1—O1W      | 3.126 (3) | O2W—H21W     | 0.7900    |
| Cs1—O2W      | 3.253 (3) | O2W—H22W     | 0.8400    |
| Cs1—O41      | 3.244 (4) | N41—C4       | 1.475 (6) |
| Cs1—O2Wi     | 3.220 (3) | C1—C2        | 1.390 (6) |
| Cs1—O42i     | 3.248 (4) | C1—C6        | 1.393 (6) |
| Cs1—O11ii    | 3.215 (3) | C1—C11       | 1.505 (7) |
| Cs1—O12ii    | 3.338 (4) | C2—C3        | 1.385 (7) |
| Cs1—O2Wiii   | 3.047 (4) | C3—C4        | 1.369 (6) |
| O11—C11      | 1.260 (6) | C5—C6        | 1.374 (6) |
| O12—C11      | 1.246 (5) | C2—H2        | 0.9500    |
| O41—N41      | 1.226 (6) | C3—H3        | 0.9500    |
| O42—N41      | 1.221 (6) | C5—H5        | 0.9500    |
| O1W—H11W     | 0.8200    | C6—H6        | 0.9500    |
| O1W—H12W     | 0.9300    |               |           |
| O1W—Cs1—O2W  | 73.36 (8) | Cs1°—O12—C11 | 87.7 (3) |
| O1W—Cs1—O41  | 134.24 (9)| Cs1°—O41—N41 | 132.6 (3) |
| O1W—Cs1—O2Wi | 72.89 (8) | Cs1°—O41—Cs1iii | 81.10 (9) |
| O1W—Cs1—O42i | 136.65 (10)| Cs1iii—O41—N41 | 135.6 (3) |
| O1W—Cs1—O11ii| 83.74 (9) | Cs1°—O42—N41 | 134.2 (3) |
| O1W—Cs1—O12i | 106.92 (9)| H11W—O1W—H12W | 110.00    |
| O1W—Cs1—O2Wiii| 129.32 (9)| Cs1°—O1W—H11W | 132.00    |
| O1W—Cs1—O41iii| 67.55 (9)| Cs1°—O1W—H12W | 104.00    |
| O2W—Cs1—O41  | 61.92 (9) | Cs1°—O2W—H21W | 94.00     |
| O2W—Cs1—O2Wi | 139.38 (9)| Cs1°—O2W—H21W | 63.00     |
| O2W—Cs1—O42i | 145.77 (10)| Cs1°—O2W—H22W | 117.00    |
| O2W—Cs1—O11i | 110.50 (8)| H21W—O2W—H22W | 105.00    |
| O2W—Cs1—O12ii| 86.77 (8) | Cs1°—O2W—H22W | 118.00    |
| O2W—Cs1—O2Wii| 94.93 (9) | Cs1°—O2W—H21W | 135.00    |
| O2W—Cs1—O41iii| 63.75 (10)| Cs1°—O2W—H22W | 101.00    |
| O2W—Cs1—O41  | 151.44 (9)| O41—N41—O42  | 123.6 (4) |
| O41—Cs1—O42i | 84.76 (11)| O42—N41—C4   | 118.2 (4) |
| O11ii—Cs1—O41| 102.41 (9)| O41—N41—C4   | 118.3 (4) |
| O12ii—Cs1—O41| 63.24 (9) | C2—C1—C11    | 120.9 (4) |
| O2W—Cs1—O41  | 66.80 (9) | C2—C1—C6     | 118.9 (4) |
| O41—Cs1—O41iii| 98.90 (10)| C6—C1—C11    | 120.1 (4) |
| O2W—Cs1—O42i | 74.49 (10)| C1—C2—C3     | 120.9 (4) |
| O2W—Cs1—O11i | 87.52 (8) | C2—C3—C4     | 117.9 (4) |
| O2W—Cs1—O12i | 124.49 (8)| C3—C4—C5     | 123.3 (4) |
| O2W—Cs1—O2Wiii| 89.33 (9) | N41—C4—C3    | 118.0 (4) |
| O2W—Cs1—O41iii| 82.79 (10)| N41—C4—C5    | 118.8 (4) |
| O11ii—Cs1—O42i| 67.02 (11)| C4—C5—C6    | 118.2 (4) |
### O12 — Cs1 — O42
- C1 — C6 — C5: 70.23 (10)
- C11 — C12 — C11: 120.9 (4)
- O11 — C11 — C12: 117.4 (4)

### O2W — Cs1 — O2W
- O11ii — C11 — O12ii: 77.45 (11)
- C1 — C2 — H2: 120.00
- C3 — C2 — H2: 120.00
- C2 — C3 — H3: 121.00

### O41 — Cs1 — O42
- O12ii — Cs1 — O12ii: 134.58 (11)
- O12ii — Cs1 — O41iii: 150.49 (9)
- O12ii — Cs1 — O41iv: 70.23 (10)

### O2W — Cs1 — O41
- C1 — C2 — H2: 120.00
- C3 — C2 — H2: 120.00
- C4 — C3 — H3: 121.00

### Cs1 — O2W — Cs1
- Cs1 — O2W — Cs1iv: 139.38 (12)
- Cs1 — O2W — Cs1iii: 85.07 (8)
- Cs1 — O2W — Cs1iv: 90.67 (9)

### Cs1 — O11 — C11
- C1 — C6 — H6: 119.00
- C5 — C6 — H6: 120.00

### O1W — Cs1 — O2W
- O1W — Cs1 — O2W — Cs1iv: −145.1 (2)
- O1W — Cs1 — O2W — Cs1iii: 129.64 (10)
- O1W — Cs1 — O2W — Cs1iv: 24.89 (16)

### O41 — Cs1 — O2W
- O41 — Cs1 — O2W — Cs1iv: −60.38 (9)
- O41 — Cs1 — O2W — Cs1iii: −179.98 (15)
- O41 — Cs1 — O2W — Cs1iv: 94.74 (13)

### O42 — Cs1 — O2W
- O42 — Cs1 — O2W — Cs1iv: 10.4 (3)
- O42 — Cs1 — O2W — Cs1iii: −74.9 (2)
- O42 — Cs1 — O2W — Cs1iv: −68.59 (19)

### O11ii — Cs1 — O2W
- O11ii — Cs1 — O2W — Cs1iv: −153.85 (8)
- O11ii — Cs1 — O2W — Cs1iii: −36.36 (18)
- O11ii — Cs1 — O2W — Cs1iv: −121.63 (9)

### O2W — Cs1 — O2W
- O2W — Cs1 — O2W — Cs1iv: 85.26 (18)
- O2W — Cs1 — O2W — Cs1iii: 0.00 (9)
- O2W — Cs1 — O2W — Cs1iv: −74.9 (2)

### O41 — Cs1 — O41
- O41 — Cs1 — O41 — Cs1iii: 78.6 (4)
- O41 — Cs1 — O41 — Cs1iv: 142.2 (2)
- O41 — Cs1 — O41 — Cs1iv: 56.92 (9)

### O1W — Cs1 — O1W
- O1W — Cs1 — O1W — Cs1iv: −79.8 (4)
- O1W — Cs1 — O1W — Cs1iii: −91.25 (19)
- O1W — Cs1 — O1W — Cs1iv: 76.23 (13)

### O2W — Cs1 — O2W
- O2W — Cs1 — O2W — Cs1iv: −93.3 (4)
- O2W — Cs1 — O2W — Cs1iii: 53.78 (9)
- O2W — Cs1 — O2W — Cs1iv: 121.7 (4)

### O2W — Cs1 — O2W
- O2W — Cs1 — O2W — Cs1iv: −91.25 (19)
- O2W — Cs1 — O2W — Cs1iii: 78.6 (4)
- O2W — Cs1 — O2W — Cs1iv: −134.36 (10)

### O1W — Cs1 — O1W
- O1W — Cs1 — O1W — Cs1iv: −145.1 (2)
- O1W — Cs1 — O1W — Cs1iii: 129.64 (10)
- O1W — Cs1 — O1W — Cs1iv: 24.89 (16)

### O2W — Cs1 — O2W
- O2W — Cs1 — O2W — Cs1iv: −60.38 (9)
- O2W — Cs1 — O2W — Cs1iii: −179.98 (15)
- O2W — Cs1 — O2W — Cs1iv: 94.74 (13)

### O41 — Cs1 — O41
- O41 — Cs1 — O41 — Cs1iii: 56.92 (9)
- O41 — Cs1 — O41 — Cs1iv: 53.78 (9)
- O41 — Cs1 — O41 — Cs1iv: 121.7 (4)

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\[
\begin{array}{cccc}
O1W—Cs1—O42^i—N41^i & -63.5 (5) & C2—C3—C4—C5 & 0.4 (7) \\
O2W—Cs1—O42^i—N41^i & 151.9 (4) & C2—C3—C4—N41 & -179.6 (4) \\
O41—Cs1—O42^i—N41^i & 139.1 (5) & C3—C4—C5—C6 & 0.1 (7) \\
O1W—Cs1—O11^ii—C11^ii & 145.7 (3) & N41—C4—C5—C6 & -180.0 (4) \\
O2W—Cs1—O11^ii—C11^ii & 76.1 (3) & C4—C5—C6—C1 & -0.7 (6) \\
O41—Cs1—O11^ii—C11^ii & 11.7 (3) & & \\
\end{array}
\]

Symmetry codes: (i) \(x-1, y, z\); (ii) \(-x+1/2, y+1/2, -z+1/2\); (iii) \(-x+1, -y, -z+1\); (iv) \(x+1, y, z\); (v) \(-x+1/2, y-1/2, -z+1/2\).

Hydrogen-bond geometry (Å, °)

\[
\begin{array}{cccccc}
D—H···A & D—H & H···A & D···A & D—H···A \\
O1W—H11W···O12^vi & 0.82 & 1.88 & 2.694 (5) & 174 \\
O1W—H12W···O11^vii & 0.93 & 1.81 & 2.728 (4) & 173 \\
O2W—H21W···O11^viii & 0.79 & 1.99 & 2.749 (5) & 162 \\
O2W—H22W···O11^vi & 0.84 & 1.91 & 2.753 (5) & 174 \\
\end{array}
\]

Symmetry codes: (vi) \(x+1/2, -y+1/2, z+1/2\); (vii) \(x-1/2, -y+1/2, z+1/2\); (viii) \(-x+1, -y+1, -z+1\).