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Tricaesium citrate monohydrate, $Cs_3C_6H_5O_7\cdot H_2O$: crystal structure and DFT comparison

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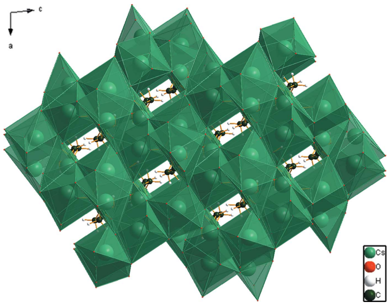
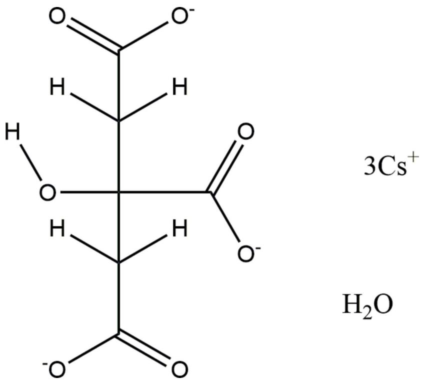
The crystal structure of tricaesium citrate monohydrate, $3Cs^+\cdot C_6H_5O_7^{3-}\cdot H_2O$, has been solved and refined using laboratory X-ray single-crystal diffraction data, and optimized using density functional techniques. This compound is isostructural to the K^+ and Rb^+ compounds with the same formula. The three independent Cs cations are eight-, eight-, and seven-coordinate, with bond-valence sums of 0.91, 1.22, and 1.12 valence units. The coordination polyhedra link into a three-dimensional framework. The hydroxy group forms the usual *S*(5) hydrogen bond with the central carboxylate group, and the water molecule acts as a donor in two strong hydrogen bonds.



1. Chemical context

In the course of a systematic study of the crystal structures of Group 1 (alkali metal) citrate salts to understand the anion's conformational flexibility, ionization, coordination tendencies, and hydrogen bonding, we have determined several new crystal structures. Most of the new structures were solved using powder diffraction data (laboratory and/or synchrotron), but single crystals were used where available. The general trends and conclusions about the sixteen new compounds and twelve previously characterized structures are being reported separately (Rammohan & Kaduk, 2017*a*). Twelve of the new structures – $NaKHC_6H_5O_7$, $NaK_2C_6H_5O_7$, $Na_3C_6H_5O_7$, $NaH_2C_6H_5O_7$, $Na_2HC_6H_5O_7$, $K_3C_6H_5O_7$, $Rb_2HC_6H_5O_7$, $Rb_3C_6H_5O_7\cdot H_2O$, $Rb_3C_6H_5O_7$, $Na_5H(C_6H_5O_7)_2$, $CsH_2C_6H_5O_7$, and $Cs_2HC_6H_5O_7$ – have been published recently (Rammohan & Kaduk, 2016*a*,*b*,*c*,*d*,*e*, 2017*b*,*c*,*d*,*e*,*f*; Rammohan *et al.*, 2016, 2017), and three additional structures – $KH_2C_6H_5O_7$ $KH_2C_6H_5O_7\cdot H_2O_2$, and $Cs_3C_6H_5O_7$ – have been communicated to the CSD (Kaduk & Stern, 2016*a*,*b*; Rammohan & Kaduk, 2017*g*).



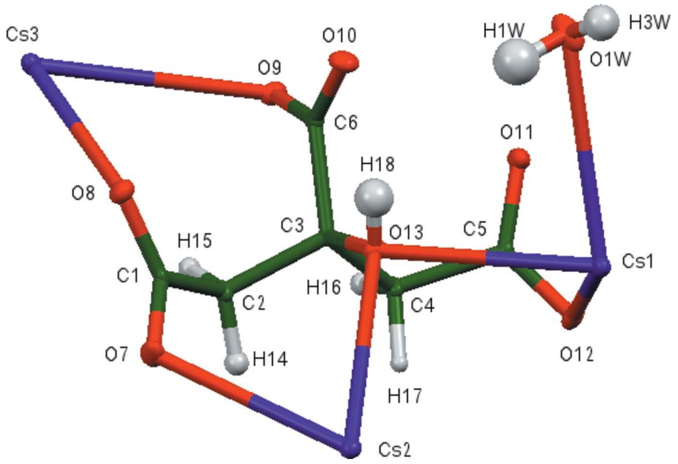


Figure 1
The asymmetric unit of the title compound, with the atom numbering. The atoms are represented by 50% probability displacement ellipsoids.

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O13—H13⋯O10	0.75 (5)	2.06 (5)	2.579 (2)	127 (4)
O1*W*—H1*WA*⋯O7^{i}	0.88 (5)	1.81 (5)	2.684 (3)	174 (5)
O1*W*—H1*WB*⋯O9^{ii}	0.76 (5)	1.95 (5)	2.695 (3)	167 (4)

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

Table 2
Hydrogen-bond geometry (Å, °) for the DFT-optimized structure.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O13—H18⋯O10	0.984	1.811	2.538	127.9
O1*W*—H1*W*⋯O7^{i}	0.984	1.719	2.686	166.8
O1*W*—H3*W*⋯O9^{ii}	0.981	1.697	2.662	167.0

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

2. Structural commentary

The asymmetric unit of the title compound is shown in Fig. 1. The root-mean-square deviation of the non-hydrogen atoms in the experimental and DFT-optimized structures is 0.123 Å (Fig. 2). The largest difference is 0.200 Å, at O1*W*. This good agreement provides strong evidence that the experimental structure is correct (van de Streek & Neumann, 2014). Almost all of the bond lengths, bond angles, and torsion angles in the experimentally determined structure fall within the normal ranges indicated by a *Mercury* Mogul geometry check (Macrae *et al.*, 2008). Only the O8—C1—C2 angle of 118.0° is flagged as unusual [average = 119.8 (4)°, Z-score = 4.2). The Z-score is the result of the exceptionally low uncertainty on the average of this bond angle. In the DFT-optimized structure, the O7—C1—C2 angle of 115.9° is flagged as unusual [average = 120.3 (12)°, Z-score = 3.6]. The citrate anion occurs in the *trans,trans* conformation, which is one of the two low-energy conformations of an isolated citrate. The three Cs^{+} cations are eight-, eight-, and seven-coordinate, with bond-valence sums of 0.91, 1.22, and 1.12 valence units. There is extensive chelation of the citrate anion to Cs^{+} cations: O12(end)/O13(OH) to Cs1, O8(end)/O10(central) to Cs2, O11(end)/O10(central) to Cs2, C11(end)/O9(central) to Cs2, O7(end)/O13(OH) to Cs2, O8(end)/O9(central) to Cs3, and O11(end)/O11(central) to Cs3. The carboxylate group O11/O12 also acts as a bidentate ligand to Cs1. The Mulliken overlap populations and atomic charges indicate that the metal–oxygen bonding is ionic.

The BFDH (Bravais–Friedel–Donnay–Harker) morphology (Bravais, 1866; Friedel, 1907; Donnay & Harker, 1937) is blocky, with {011} as major faces. The powder pattern exhibited strong preferred orientation consistent with {101} as the major faces of plates. These faces are also significant in the BFDH morphology.

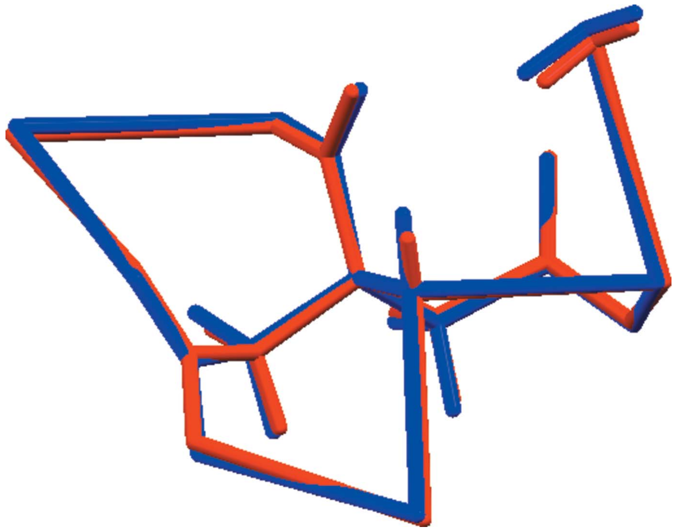


Figure 2
Comparison of the refined and optimized structures of tricaesium citrate monohydrate. The refined structure is in red and the DFT-optimized structure is in blue.

3. Supramolecular features

The coordination polyhedra link into a three-dimensional framework (Fig. 3). The hydrophobic methylene groups occupy pockets in the framework. The hydroxy group forms the usual *S*(5) hydrogen bond with the central carboxylate group, and the water molecule acts as a donor in two strong hydrogen bonds (2.686 and 2.662 Å). By the correlation between the square root of the Mulliken overlap population and hydrogen-bond energy derived in Rammohan & Kaduk (2017*a*), these hydrogen bonds contribute 14.4, 14.1, and 14.1 kcal mol^{-1}, respectively, to the crystal energy. Numerical details of the hydrogen bonds in the experimentally determined and DFT-optimized structures are given in Tables 1 and 2, respectively.

4. Database survey

Details of the comprehensive literature search for citrate structures are presented in Rammohan & Kaduk (2017*a*). A

Table 3
Lattice parameters (Å, °, Å^3, K; space group $P2_1/n$) of $M_3C_6H_5O_7 \cdot H_2O$.

	K[a]	Rb[b]	Cs[c]
a	7.092 (2)	7.4477 (1)	7.88551 (4)
b	11.772 (1)	11.8755 (2)	12.2109 (8)
c	12.865 (1)	13.4167 (2)	14.0367 (8)
β	98.031 (2)	97.8820 (9)	97.280 (4)
V	1063.50	1175.44 (3)	1340.63 (14)
V/non-H	16.6	17.3	19.7
T	300	300	100

References: (*a*) Carrell *et al.* (1987); (*b*) Rammohan & Kaduk (2017*c*); (*c*) this work.

reduced-cell search of the cell of tricaesium citrate monohydrate in the Cambridge Structural Database (Groom *et al.*, 2016) (increasing the default tolerance from 1.5 to 2.0%) yielded 258 hits, but combining the cell search with the elements C, H, Cs, and O only yielded no hits. Increasing the tolerance to 5% with C, H, O, and Rb only yielded trirubidium citrate monohydrate (Love & Patterson, 1960; CSD refcode ZZZHZC), but no coordinates were reported for this phase. The structure has since been reported by Rammohan & Kaduk (2017*c*). Increasing the tolerance on the cell to 7% with C, H, K, and O only yielded $K_3C_6H_5O_7 \cdot H_2O$ (Burns & Iball, 1954, CSD refcode ZZZHVI; Carrell *et al.*, 1987, CSD refcodes ZZZHVI01 and ZZZHVI02). This compound is isostructural to the K$^+$ (Carrell *et al.*, 1987) and Rb$^+$ (Rammohan & Kaduk, 2017*c*) compounds with the same formula, but the previously-reported structure of $K_3C_6H_5O_7 \cdot H_2O$ has to be transformed from setting $P2_1/a$ to $P2_1/n$ to make the similarities clear (Table 3).

5. Synthesis and crystallization

$H_3C_6H_5O_7 \cdot H_2O$ (2.0774 g, 10.0 mmol, Sigma–Aldrich) was dissolved in 8 ml deionized water. Cs_2CO_3 (4.9324 g, 15.1 mmole, Sigma–Aldrich) was added to the citric acid solution slowly with stirring. The resulting clear colorless solution was evaporated to dryness in a oven at 333 K. Single crystals were isolated from the white product.

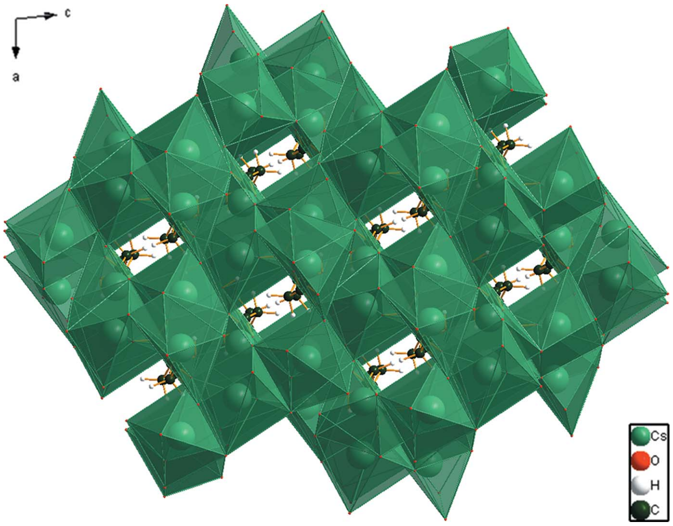


Figure 3
Crystal structure of $Cs_3C_6H_5O_7 \cdot H_2O$, viewed down the *b* axis.

Table 4
Experimental details.

	X-ray data
Crystal data	
Chemical formula	$3Cs^+ \cdot C_6H_5O_7^{3-} \cdot H_2O$
M_r	605.85
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, *b*, *c* (Å)	7.7529 (3), 12.0281 (4), 13.8043 (5)
β (°)	97.000 (2)
V (Å^3)	1277.69 (8)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	8.54
Crystal size (mm)	0.37 × 0.28 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEX CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.485, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33171, 6191, 5701
R_{int}	0.040
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.834
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.047, 1.16
No. of reflections	6191
No. of parameters	183
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.41, −1.19

The same symmetry and lattice parameters were used for the DFT calculations. Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *XM* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. The hydrogen atoms were freely refined with isotropic ADPs. The lattice parameters at 300 K (derived from a Le Bail fit of the powder pattern) are a = 7.8851 (4), b = 12.2109 (8), c = 14.0367 (8) Å, β = 97.280 (4)°, and V = 1340.63 (14) Å^3.

7. DFT calculations

After the Rietveld refinement, a density functional geometry optimization (fixed experimental unit cell at 100 K) was carried out using *CRYSTAL09* (Dovesi *et al.*, 2005). The basis sets for the C, H, and O atoms were those of Gatti *et al.* (1994), and the basis set for Cs was that of Prencipe (1990). The calculation used 8 *k*-points and the B3LYP functional, and took about 85 h on a 2.4 GHz PC. The U_{eq} values from the refinement were assigned to the optimized fractional coordinates.

Acknowledgements

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supporting information

Acta Cryst. (2017). E**73**, 520-523   [https://doi.org/10.1107/S205698901700367X]

Tricaesium citrate monohydrate, $Cs_3C_6H_5O_7\cdot H_2O$: crystal structure and DFT comparison

Alagappa Rammohan, Amy A. Sarjeant and James A. Kaduk

Computing details

Data collection: *APEX2* (Bruker, 2008) for (I). Cell refinement: *SAINT* (Bruker, 2008) for (I). Data reduction: *SAINT* (Bruker, 2008) for (I). Program(s) used to solve structure: XM (Sheldrick, 2008) for (I); DFT calculation for I_DFT. Program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015) for (I). Molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) for (I). Software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009) for (I).

(I) Tricaesium citrate monohydrate

Crystal data

$3Cs^+\cdot C_6H_5O_7^{3-}\cdot H_2O$
$M_r = 605.85$
Monoclinic, $P2_1/n$
$a = 7.7529$ (3) Å
$b = 12.0281$ (4) Å
$c = 13.8043$ (5) Å
$\beta = 97.000$ (2)°
$V = 1277.69$ (8) Å^3
$Z = 4$

$F(000) = 1088$
$D_x = 3.150$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9882 reflections
$\theta = 2.3$–$36.3°$
$\mu = 8.54$ mm^{-1}
$T = 100$ K
Block, colourless
0.37 × 0.28 × 0.20 mm

Data collection

Bruker Kappa APEX CCD area detector diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
$T_{min} = 0.485$, $T_{max} = 0.747$

33171 measured reflections
6191 independent reflections
5701 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 36.4°$, $\theta_{min} = 2.3°$
$h = -12 \rightarrow 12$
$k = -20 \rightarrow 20$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.047$
$S = 1.16$
6191 reflections
183 parameters
0 restraints

Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0103P)^2 + 1.2602P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.41$ e Å^{-3}
$\Delta\rho_{min} = -1.19$ e Å^{-3}

Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00244 (9)

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{\rm iso}*/U_{\rm eq}$
Cs1	0.51414 (2)	0.83481 (2)	0.61851 (2)	0.00997 (3)
Cs2	0.84130 (2)	0.56550 (2)	0.61084 (2)	0.00900 (3)
Cs3	0.38447 (2)	0.43247 (2)	0.11056 (2)	0.01111 (3)
O1W	0.1171 (3)	0.78232 (16)	0.55701 (16)	0.0189 (4)
H1WA	0.165 (6)	0.716 (4)	0.565 (4)	0.041 (12)*
O7	0.7546 (2)	0.42499 (14)	0.42718 (13)	0.0149 (3)
O8	0.5102 (2)	0.42227 (13)	0.32357 (13)	0.0121 (3)
O9	0.4043 (2)	0.68462 (13)	0.19483 (12)	0.0112 (3)
O10	0.2781 (2)	0.66791 (14)	0.33147 (13)	0.0127 (3)
O11	0.4663 (2)	0.91616 (13)	0.32807 (14)	0.0135 (3)
O12	0.7007 (2)	0.94370 (14)	0.43602 (14)	0.0162 (3)
O13	0.5640 (2)	0.66687 (13)	0.44855 (12)	0.0101 (3)
H13	0.470 (6)	0.652 (4)	0.448 (3)	0.034 (12)*
C1	0.6500 (3)	0.46607 (17)	0.35969 (16)	0.0086 (3)
C2	0.6996 (3)	0.57813 (16)	0.31910 (17)	0.0091 (3)
H2A	0.820 (4)	0.592 (3)	0.346 (2)	0.011 (7)*
H2B	0.689 (5)	0.577 (3)	0.252 (3)	0.011 (8)*
C3	0.5887 (3)	0.67637 (16)	0.34819 (15)	0.0075 (3)
C4	0.6931 (3)	0.78262 (17)	0.33527 (17)	0.0101 (3)
H4A	0.718 (4)	0.790 (3)	0.268 (3)	0.012 (8)*
H4B	0.808 (4)	0.773 (3)	0.380 (2)	0.008 (7)*
C5	0.6133 (3)	0.88902 (16)	0.36962 (15)	0.0084 (3)
C6	0.4075 (3)	0.67732 (16)	0.28626 (16)	0.0083 (3)
H1WB	0.070 (6)	0.790 (3)	0.602 (3)	0.027 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs1	0.00914 (6)	0.00735 (5)	0.01319 (6)	0.00069 (4)	0.00047 (4)	−0.00094 (4)
Cs2	0.00823 (5)	0.00929 (5)	0.00945 (6)	−0.00067 (4)	0.00095 (4)	−0.00012 (4)
Cs3	0.01091 (6)	0.01313 (6)	0.00897 (6)	0.00360 (4)	−0.00008 (4)	−0.00176 (4)
O1W	0.0224 (9)	0.0138 (8)	0.0229 (9)	0.0050 (7)	0.0124 (8)	0.0086 (7)
O7	0.0170 (8)	0.0115 (7)	0.0147 (8)	0.0051 (6)	−0.0045 (6)	−0.0001 (6)
O8	0.0123 (7)	0.0108 (7)	0.0128 (7)	−0.0024 (5)	0.0004 (6)	−0.0005 (5)
O9	0.0113 (7)	0.0140 (7)	0.0083 (7)	−0.0017 (5)	0.0009 (5)	0.0010 (5)

O10	0.0079 (7)	0.0160 (7)	0.0147 (8)	−0.0001 (5)	0.0031 (6)	0.0026 (6)
O11	0.0103 (7)	0.0108 (7)	0.0185 (8)	0.0014 (5)	−0.0013 (6)	−0.0029 (6)
O12	0.0175 (8)	0.0117 (7)	0.0174 (8)	0.0005 (6)	−0.0060 (7)	−0.0053 (6)
O13	0.0097 (7)	0.0122 (7)	0.0085 (7)	−0.0008 (5)	0.0014 (5)	−0.0007 (5)
C1	0.0102 (8)	0.0064 (7)	0.0094 (8)	0.0023 (6)	0.0016 (7)	−0.0014 (6)
C2	0.0081 (8)	0.0065 (7)	0.0131 (9)	0.0005 (6)	0.0037 (7)	−0.0002 (6)
C3	0.0082 (8)	0.0062 (7)	0.0080 (8)	−0.0001 (6)	0.0000 (6)	0.0005 (6)
C4	0.0084 (8)	0.0074 (8)	0.0147 (9)	−0.0007 (6)	0.0020 (7)	−0.0014 (7)
C5	0.0112 (8)	0.0065 (7)	0.0077 (8)	−0.0015 (6)	0.0019 (7)	0.0002 (6)
C6	0.0088 (8)	0.0054 (7)	0.0105 (8)	−0.0005 (6)	0.0005 (7)	0.0002 (6)

Geometric parameters (Å, º)

Cs1—O1W	3.156 (2)	O7—C1	1.259 (3)
Cs1—O7^{i}	3.7660 (18)	O8—Cs1^{i}	3.2051 (16)
Cs1—O8^{i}	3.2052 (16)	O8—Cs2^{i}	2.9783 (18)
Cs1—O9^{ii}	3.0886 (17)	O8—C1	1.252 (3)
Cs1—O10^{ii}	3.3711 (18)	O9—Cs1^{vii}	3.0886 (17)
Cs1—O11^{iii}	3.0842 (16)	O9—Cs2^{vii}	3.2371 (16)
Cs1—O12^{iii}	3.1834 (18)	O9—C6	1.262 (3)
Cs1—O12	3.323 (2)	O10—Cs1^{vii}	3.3711 (18)
Cs1—O13	3.1552 (16)	O10—Cs2^{i}	3.0906 (17)
Cs2—O1W^{iv}	3.5088 (19)	O10—Cs3^{x}	3.5497 (17)
Cs2—O7	3.0529 (18)	O10—C6	1.250 (3)
Cs2—O7^{v}	3.241 (2)	O11—Cs1^{iii}	3.0842 (16)
Cs2—O8^{i}	2.9782 (18)	O11—Cs2^{vii}	3.0449 (18)
Cs2—O9^{ii}	3.2371 (16)	O11—Cs3^{x}	2.9519 (18)
Cs2—O10^{i}	3.0906 (17)	O11—C5	1.255 (3)
Cs2—O11^{ii}	3.0450 (18)	O12—Cs1^{iii}	3.1834 (17)
Cs2—O13	3.1551 (17)	O12—Cs3^{xi}	3.358 (2)
Cs3—O1W^{vi}	2.9336 (19)	O12—Cs3^{ii}	3.0358 (17)
Cs3—O8	2.9855 (17)	O12—C5	1.257 (3)
Cs3—O9	3.2452 (16)	O13—H13	0.75 (5)
Cs3—O10^{vi}	3.5497 (17)	O13—C3	1.426 (3)
Cs3—O11^{vi}	2.9519 (18)	C1—C2	1.527 (3)
Cs3—O12^{vii}	3.0358 (17)	C2—H2A	0.98 (3)
Cs3—O12^{viii}	3.358 (2)	C2—H2B	0.91 (3)
O1W—Cs2^{ix}	3.5088 (19)	C2—C3	1.543 (3)
O1W—Cs3^{x}	2.9336 (19)	C3—C4	1.535 (3)
O1W—H1WA	0.88 (5)	C3—C6	1.553 (3)
O1W—H1WB	0.76 (5)	C4—H4A	0.98 (4)
O7—Cs1^{i}	3.7660 (18)	C4—H4B	1.03 (3)
O7—Cs2^{v}	3.2412 (19)	C4—C5	1.522 (3)

O1W—Cs1—O7^{i}	44.55 (4)	C1—O7—Cs2	117.00 (13)
O1W—Cs1—O8^{i}	77.81 (5)	Cs2^{i}—O8—Cs1^{i}	83.57 (4)
O1W—Cs1—O10^{ii}	134.52 (5)	Cs2^{i}—O8—Cs3	95.53 (5)
O1W—Cs1—O12^{iii}	68.81 (5)	Cs3—O8—Cs1^{i}	105.26 (5)

O1W—Cs1—O12	112.05 (5)	C1—O8—Cs1^{i}	112.39 (13)
O8^{i}—Cs1—O7^{i}	36.20 (4)	C1—O8—Cs2^{i}	129.60 (14)
O8^{i}—Cs1—O10^{ii}	79.69 (4)	C1—O8—Cs3	122.53 (14)
O8^{i}—Cs1—O12	127.85 (4)	Cs1^{vii}—O9—Cs2^{vii}	81.33 (4)
O9^{ii}—Cs1—O1W	163.62 (5)	Cs1^{vii}—O9—Cs3	78.77 (4)
O9^{ii}—Cs1—O7^{i}	119.55 (4)	Cs2^{vii}—O9—Cs3	137.80 (5)
O9^{ii}—Cs1—O8^{i}	85.81 (4)	C6—O9—Cs1^{vii}	103.57 (13)
O9^{ii}—Cs1—O10^{ii}	40.24 (4)	C6—O9—Cs2^{vii}	113.98 (12)
O9^{ii}—Cs1—O12	77.85 (4)	C6—O9—Cs3	106.72 (12)
O9^{ii}—Cs1—O12^{iii}	127.34 (4)	Cs1^{vii}—O10—Cs3^{x}	90.62 (4)
O9^{ii}—Cs1—O13	90.09 (4)	Cs2^{i}—O10—Cs1^{vii}	92.69 (4)
O10^{ii}—Cs1—O7^{i}	113.74 (4)	Cs2^{i}—O10—Cs3^{x}	129.09 (5)
O11^{iii}—Cs1—O1W	106.05 (5)	C6—O10—Cs1^{vii}	90.25 (13)
O11^{iii}—Cs1—O7^{i}	148.87 (4)	C6—O10—Cs2^{i}	119.66 (13)
O11^{iii}—Cs1—O8^{i}	151.64 (5)	C6—O10—Cs3^{x}	111.11 (13)
O11^{iii}—Cs1—O9^{ii}	88.53 (4)	Cs2^{vii}—O11—Cs1^{iii}	99.53 (5)
O11^{iii}—Cs1—O10^{ii}	78.11 (4)	Cs3^{x}—O11—Cs1^{iii}	83.51 (4)
O11^{iii}—Cs1—O12	77.60 (5)	Cs3^{x}—O11—Cs2^{vii}	94.82 (5)
O11^{iii}—Cs1—O12^{iii}	41.65 (4)	C5—O11—Cs1^{iii}	97.35 (12)
O11^{iii}—Cs1—O13	142.44 (5)	C5—O11—Cs2^{vii}	129.15 (14)
O12—Cs1—O7^{i}	118.89 (4)	C5—O11—Cs3^{x}	134.67 (15)
O12^{iii}—Cs1—O7^{i}	113.07 (4)	Cs1^{iii}—O12—Cs1	104.21 (6)
O12^{iii}—Cs1—O8^{i}	145.22 (5)	Cs1^{iii}—O12—Cs3^{xi}	118.30 (6)
O12^{iii}—Cs1—O10^{ii}	117.31 (4)	Cs1—O12—Cs3^{xi}	130.15 (6)
O12—Cs1—O10^{ii}	113.01 (4)	Cs3^{ii}—O12—Cs1	78.30 (4)
O12^{iii}—Cs1—O12	75.79 (6)	Cs3^{ii}—O12—Cs1^{iii}	87.62 (4)
O13—Cs1—O1W	82.86 (5)	Cs3^{ii}—O12—Cs3^{xi}	78.70 (4)
O13—Cs1—O7^{i}	57.29 (4)	C5—O12—Cs1^{iii}	92.59 (13)
O13—Cs1—O8^{i}	65.43 (4)	C5—O12—Cs1	95.77 (14)
O13—Cs1—O10^{ii}	121.73 (4)	C5—O12—Cs3^{ii}	173.92 (16)
O13—Cs1—O12^{iii}	117.90 (4)	C5—O12—Cs3^{xi}	106.46 (14)
O13—Cs1—O12	65.45 (4)	Cs1—O13—H13	87 (4)
O7—Cs2—O1W^{iv}	108.29 (5)	Cs2—O13—Cs1	81.61 (4)
O7^{v}—Cs2—O1W^{iv}	46.65 (4)	Cs2—O13—H13	120 (3)
O7—Cs2—O7^{v}	90.26 (5)	C3—O13—Cs1	135.57 (12)
O7—Cs2—O9^{ii}	145.06 (4)	C3—O13—Cs2	124.07 (12)
O7—Cs2—O10^{i}	70.65 (5)	C3—O13—H13	105 (4)
O7—Cs2—O13	64.04 (4)	Cs1^{i}—C1—Cs2^{i}	64.22 (3)
O8^{i}—Cs2—O1W^{iv}	129.16 (5)	Cs2—C1—Cs1^{i}	108.67 (5)
O8^{i}—Cs2—O7^{v}	170.36 (5)	Cs2—C1—Cs2^{i}	102.33 (5)
O8^{i}—Cs2—O7	99.37 (5)	Cs2—C1—Cs3	165.18 (6)
O8^{i}—Cs2—O9^{ii}	87.08 (4)	Cs3—C1—Cs1^{i}	79.86 (4)
O8^{i}—Cs2—O10^{i}	69.68 (4)	Cs3—C1—Cs2^{i}	69.91 (4)
O8^{i}—Cs2—O11^{ii}	83.70 (5)	O7—C1—Cs1^{i}	76.30 (12)
O8^{i}—Cs2—O13	68.11 (5)	O7—C1—Cs2^{i}	115.73 (15)
O9^{ii}—Cs2—O1W^{iv}	46.88 (5)	O7—C1—Cs2	45.80 (11)
O9^{ii}—Cs2—O7^{v}	85.32 (4)	O7—C1—Cs3	148.76 (14)
O10^{i}—Cs2—O1W^{iv}	159.89 (5)	O7—C1—C2	116.69 (19)

O10^{i}—Cs2—O7^{v}	113.55 (4)	O8—C1—Cs1^{i}	50.15 (11)
O10^{i}—Cs2—O9^{ii}	142.00 (4)	O8—C1—Cs2^{i}	36.07 (11)
O10^{i}—Cs2—O13	109.54 (4)	O8—C1—Cs2	136.00 (15)
O11^{ii}—Cs2—O1W^{iv}	91.47 (5)	O8—C1—Cs3	41.38 (11)
O11^{ii}—Cs2—O7^{v}	87.65 (5)	O8—C1—O7	125.3 (2)
O11^{ii}—Cs2—O7	150.39 (4)	O8—C1—C2	118.03 (19)
O11^{ii}—Cs2—O9^{ii}	64.15 (4)	C1—C2—H2A	106.6 (19)
O11^{ii}—Cs2—O10^{i}	83.19 (4)	C1—C2—H2B	111 (2)
O11^{ii}—Cs2—O13	141.15 (4)	C1—C2—C3	114.00 (17)
O13—Cs2—O1W^{iv}	86.70 (5)	H2A—C2—H2B	111 (3)
O13—Cs2—O7^{v}	117.38 (5)	C3—C2—H2A	107.6 (19)
O13—Cs2—O9^{ii}	87.46 (4)	C3—C2—H2B	107 (2)
O1W^{vi}—Cs3—O8	136.12 (5)	O13—C3—C2	109.66 (16)
O1W^{vi}—Cs3—O9	148.59 (5)	O13—C3—C4	108.35 (17)
O1W^{vi}—Cs3—O10^{vi}	70.03 (5)	O13—C3—C6	108.42 (17)
O1W^{vi}—Cs3—O11^{vi}	105.66 (5)	C2—C3—C6	110.97 (17)
O1W^{vi}—Cs3—O12^{viii}	77.63 (5)	C4—C3—C2	106.76 (17)
O1W^{vi}—Cs3—O12^{vii}	73.73 (6)	C4—C3—C6	112.62 (16)
O8—Cs3—O9	71.93 (4)	C3—C4—H4A	111 (2)
O8—Cs3—O10^{vi}	79.83 (4)	C3—C4—H4B	105.7 (18)
O8—Cs3—O12^{viii}	89.13 (5)	H4A—C4—H4B	109 (3)
O8—Cs3—O12^{vii}	150.13 (5)	C5—C4—C3	115.05 (18)
O9—Cs3—O10^{vi}	139.43 (4)	C5—C4—H4A	111 (2)
O9—Cs3—O12^{viii}	91.51 (4)	C5—C4—H4B	105.0 (18)
O11^{vi}—Cs3—O8	85.20 (5)	O11—C5—Cs1^{iii}	61.67 (11)
O11^{vi}—Cs3—O9	87.96 (4)	O11—C5—Cs1	101.08 (14)
O11^{vi}—Cs3—O10^{vi}	60.72 (4)	O11—C5—Cs3^{xi}	147.07 (14)
O11^{vi}—Cs3—O12^{viii}	174.19 (5)	O11—C5—O12	125.2 (2)
O11^{vi}—Cs3—O12^{vii}	84.31 (5)	O11—C5—C4	117.22 (18)
O12^{vii}—Cs3—O9	79.81 (4)	O12—C5—Cs1	64.30 (13)
O12^{vii}—Cs3—O10^{vi}	118.27 (4)	O12—C5—Cs1^{iii}	66.22 (12)
O12^{viii}—Cs3—O10^{vi}	116.99 (4)	O12—C5—Cs3^{xi}	55.55 (13)
O12^{vii}—Cs3—O12^{viii}	101.30 (4)	O12—C5—C4	117.59 (19)
Cs1—O1W—Cs2^{ix}	133.73 (6)	O9—C6—Cs1^{vii}	56.50 (11)
Cs3^{x}—O1W—Cs1	89.95 (5)	O9—C6—Cs2^{i}	118.05 (13)
Cs3^{x}—O1W—Cs2^{ix}	132.88 (7)	O9—C6—Cs3	54.76 (10)
H1WA—O1W—H1WB	104 (4)	O9—C6—C3	117.20 (19)
Cs2^{v}—O7—Cs1^{i}	121.88 (5)	O10—C6—Cs1^{vii}	69.44 (12)
Cs2—O7—Cs1^{i}	131.28 (6)	O10—C6—Cs2^{i}	44.02 (11)
Cs2—O7—Cs2^{v}	89.74 (5)	O10—C6—Cs3	105.67 (13)
C1—O7—Cs1^{i}	84.74 (13)	O10—C6—O9	125.9 (2)
C1—O7—Cs2^{v}	114.49 (15)	O10—C6—C3	116.86 (19)

Cs1^{i}—O7—C1—Cs2	134.16 (11)	Cs2^{vii}—O11—C5—C4	−50.2 (3)
Cs1^{i}—O7—C1—Cs2^{i}	52.09 (9)	Cs2—O13—C3—C2	33.2 (2)
Cs1^{i}—O7—C1—Cs3	−41.3 (3)	Cs2—O13—C3—C4	−83.01 (17)
Cs1^{i}—O7—C1—O8	11.4 (2)	Cs2—O13—C3—C6	154.48 (11)
Cs1^{i}—O7—C1—C2	−168.34 (17)	Cs2—C1—C2—C3	−70.94 (16)

Cs1^{i}—O8—C1—Cs2^{i}	−100.58 (17)	Cs2^{i}—C1—C2—C3	31.8 (2)
Cs1^{i}—O8—C1—Cs2	−74.70 (19)	Cs3—O8—C1—Cs1^{i}	−126.90 (16)
Cs1^{i}—O8—C1—Cs3	126.90 (16)	Cs3—O8—C1—Cs2^{i}	132.5 (2)
Cs1^{i}—O8—C1—O7	−14.5 (3)	Cs3—O8—C1—Cs2	158.40 (9)
Cs1^{i}—O8—C1—C2	165.25 (14)	Cs3—O8—C1—O7	−141.38 (18)
Cs1^{vii}—O9—C6—Cs2^{i}	49.76 (13)	Cs3—O8—C1—C2	38.3 (2)
Cs1^{vii}—O9—C6—Cs3	82.15 (7)	Cs3—O9—C6—Cs1^{vii}	−82.15 (7)
Cs1^{vii}—O9—C6—O10	−1.9 (2)	Cs3—O9—C6—Cs2^{i}	−32.38 (14)
Cs1^{vii}—O9—C6—C3	176.14 (13)	Cs3—O9—C6—O10	−84.1 (2)
Cs1^{vii}—O10—C6—Cs2^{i}	−93.24 (11)	Cs3—O9—C6—C3	93.99 (16)
Cs1^{vii}—O10—C6—Cs3	−55.83 (7)	Cs3^{x}—O10—C6—Cs1^{vii}	−90.76 (8)
Cs1^{vii}—O10—C6—O9	1.7 (2)	Cs3^{x}—O10—C6—Cs2^{i}	176.00 (17)
Cs1^{vii}—O10—C6—C3	−176.35 (15)	Cs3^{x}—O10—C6—Cs3	−146.59 (6)
Cs1^{iii}—O11—C5—Cs1	86.11 (7)	Cs3^{x}—O10—C6—O9	−89.1 (2)
Cs1^{iii}—O11—C5—Cs3^{xi}	−59.5 (3)	Cs3^{x}—O10—C6—C3	92.88 (17)
Cs1^{iii}—O11—C5—O12	19.9 (2)	Cs3^{x}—O11—C5—Cs1	−2.01 (19)
Cs1^{iii}—O11—C5—C4	−158.83 (16)	Cs3^{x}—O11—C5—Cs1^{iii}	−88.12 (15)
Cs1^{iii}—O12—C5—Cs1	−104.57 (7)	Cs3^{x}—O11—C5—Cs3^{xi}	−147.63 (15)
Cs1—O12—C5—Cs1^{iii}	104.57 (7)	Cs3^{x}—O11—C5—O12	−68.3 (3)
Cs1—O12—C5—Cs3^{xi}	−134.88 (9)	Cs3^{x}—O11—C5—C4	113.0 (2)
Cs1^{iii}—O12—C5—Cs3^{xi}	120.55 (9)	Cs3^{xi}—O12—C5—Cs1	134.88 (9)
Cs1—O12—C5—O11	85.5 (2)	Cs3^{xi}—O12—C5—Cs1^{iii}	−120.55 (9)
Cs1^{iii}—O12—C5—O11	−19.1 (2)	Cs3^{xi}—O12—C5—O11	−139.6 (2)
Cs1—O12—C5—C4	−95.82 (18)	Cs3^{xi}—O12—C5—C4	39.1 (2)
Cs1^{iii}—O12—C5—C4	159.61 (16)	Cs3—C1—C2—C3	96.43 (16)
Cs1—O13—C3—C2	149.16 (14)	Cs3^{xi}—C4—C5—Cs1	−102.19 (7)
Cs1—O13—C3—C4	33.0 (2)	Cs3^{xi}—C4—C5—Cs1^{iii}	64.1 (4)
Cs1—O13—C3—C6	−89.54 (19)	Cs3^{xi}—C4—C5—O11	145.71 (18)
Cs1^{i}—C1—C2—C3	114.1 (4)	Cs3^{xi}—C4—C5—O12	−33.08 (19)
Cs2—O7—C1—Cs1^{i}	−134.16 (11)	O7—C1—C2—C3	−108.2 (2)
Cs2^{v}—O7—C1—Cs1^{i}	122.74 (9)	O8—C1—C2—C3	72.1 (3)
Cs2—O7—C1—Cs2^{i}	−82.07 (14)	O13—C3—C4—Cs3^{xi}	66.8 (3)
Cs2^{v}—O7—C1—Cs2	−103.10 (14)	O13—C3—C4—C5	−56.4 (2)
Cs2^{v}—O7—C1—Cs2^{i}	174.83 (5)	O13—C3—C6—Cs2^{i}	−46.78 (15)
Cs2—O7—C1—Cs3	−175.46 (19)	O13—C3—C6—Cs3	−120.44 (13)
Cs2^{v}—O7—C1—Cs3	81.4 (3)	O13—C3—C6—O9	−179.56 (17)
Cs2—O7—C1—O8	−122.8 (2)	O13—C3—C6—O10	−1.3 (2)
Cs2^{v}—O7—C1—O8	134.14 (19)	C1—C2—C3—O13	42.5 (2)
Cs2—O7—C1—C2	57.5 (2)	C1—C2—C3—C4	159.72 (18)
Cs2^{v}—O7—C1—C2	−45.6 (2)	C1—C2—C3—C6	−77.2 (2)
Cs2^{i}—O8—C1—Cs1^{i}	100.58 (17)	C2—C3—C4—Cs3^{xi}	−51.3 (3)
Cs2^{i}—O8—C1—Cs2	25.9 (3)	C2—C3—C4—C5	−174.41 (18)
Cs2^{i}—O8—C1—Cs3	−132.5 (2)	C2—C3—C6—Cs2^{i}	73.71 (16)
Cs2^{i}—O8—C1—O7	86.1 (3)	C2—C3—C6—Cs3	0.05 (18)
Cs2^{i}—O8—C1—C2	−94.2 (2)	C2—C3—C6—O9	−59.1 (2)
Cs2^{vii}—O9—C6—Cs1^{vii}	86.42 (9)	C2—C3—C6—O10	119.2 (2)
Cs2^{vii}—O9—C6—Cs2^{i}	136.19 (7)	C3—C4—C5—Cs1	50.77 (19)
Cs2^{vii}—O9—C6—Cs3	168.57 (14)	C3—C4—C5—Cs1^{iii}	−143.0 (4)

Cs2^{vii}—O9—C6—O10	84.5 (2)	C3—C4—C5—Cs3^{xi}	152.96 (19)
Cs2^{vii}—O9—C6—C3	−97.44 (17)	C3—C4—C5—O11	−61.3 (3)
Cs2^{i}—O10—C6—Cs1^{vii}	93.24 (11)	C3—C4—C5—O12	119.9 (2)
Cs2^{i}—O10—C6—Cs3	37.41 (15)	C4—C3—C6—Cs2^{i}	−166.67 (13)
Cs2^{i}—O10—C6—O9	94.9 (2)	C4—C3—C6—Cs3	119.68 (15)
Cs2^{i}—O10—C6—C3	−83.12 (19)	C4—C3—C6—O9	60.6 (2)
Cs2^{vii}—O11—C5—Cs1	−165.21 (9)	C4—C3—C6—O10	−121.2 (2)
Cs2^{vii}—O11—C5—Cs1^{iii}	108.68 (15)	C6—C3—C4—Cs3^{xi}	−173.29 (18)
Cs2^{vii}—O11—C5—Cs3^{xi}	49.2 (3)	C6—C3—C4—C5	63.6 (2)
Cs2^{vii}—O11—C5—O12	128.5 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O13—H13···O10	0.75 (5)	2.06 (5)	2.579 (2)	127 (4)
O1*W*—H1*WA*···O7^{i}	0.88 (5)	1.81 (5)	2.684 (3)	174 (5)
O1*W*—H1*WB*···O9^{xii}	0.76 (5)	1.95 (5)	2.695 (3)	167 (4)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (xii) *x*−1/2, −*y*+3/2, *z*+1/2.

(I_DFT) Tricaesium citrate monohydrate

Crystal data

$3Cs^{+}\cdot C_6H_5O_7^{3-}\cdot H_2O$
M_r = 605.85
Monoclinic, $P2_1/n$
a = 7.7529 Å
b = 12.0281 Å
c = 13.8043 Å
β = 97.0000°
V = 1277.69 Å^3
Z = 4
DFT calculation radiation, *λ* = 1.54184 Å
T = 100 K

Data collection

h = →
k = →
l = →

Refinement

H-atom parameters not refined

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cs1	0.50780	0.82708	0.61694	0.00960*
Cs2	0.83209	0.55810	0.61104	0.00867*
Cs3	0.38395	0.43445	0.11206	0.01077*
O7	0.78685	0.43530	0.42471	0.01460*
O8	0.53202	0.41899	0.32856	0.01190*
O9	0.40939	0.69538	0.19097	0.01090*
O10	0.28355	0.67716	0.32774	0.01250*
O11	0.46920	0.91349	0.32953	0.01330*
O12	0.71297	0.95547	0.42842	0.01600*

O13	0.56194	0.66231	0.44450	0.00980*
H18	0.43476	0.65343	0.43651	0.02800*
C1	0.67041	0.46915	0.35846	0.00830*
C2	0.70544	0.58130	0.31182	0.00870*
H14	0.84281	0.60200	0.33092	0.01100*
H15	0.68245	0.57527	0.23228	0.00900*
C3	0.59503	0.67849	0.34578	0.00720*
C4	0.70484	0.78402	0.34170	0.00980*
H16	0.74216	0.79325	0.26803	0.01000*
H17	0.82267	0.77093	0.39247	0.00600*
C5	0.62112	0.89281	0.36933	0.00800*
C6	0.41465	0.68598	0.28244	0.00790*
O1W	0.09706	0.77363	0.54410	0.01850*
H1W	0.14970	0.69912	0.54760	0.04000*
H3W	0.04287	0.78150	0.60432	0.02400*

Bond lengths (Å)

O7—C1	1.271	C2—H15	1.093
O8—C1	1.256	C2—C3	1.555
O9—C6	1.263	C3—C4	1.533
O10—C6	1.261	C3—C6	1.559
O11—C5	1.262	C4—H16	1.096
O12—C5	1.264	C4—H17	1.093
O13—H18	0.984	C4—C5	1.529
O13—C3	1.430	O1W—H1W	0.984
C1—C2	1.533	O1W—H3W	0.981
C2—H14	1.094		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O13—H18···O10	0.984	1.811	2.538	127.9
O1*W*—H1*W*···O7^{i}	0.984	1.719	2.686	166.8
O1*W*—H3*W*···O9^{ii}	0.981	1.697	2.662	167.0

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x-1/2, -y+3/2, z+1/2$.