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catena-Poly[[diaquacalcium]bis[μ-2-(1,3-dioxoisoindolin-2-yl)acetato]-$\kappa^3O,O':O;\kappa^3O:O,O'$]

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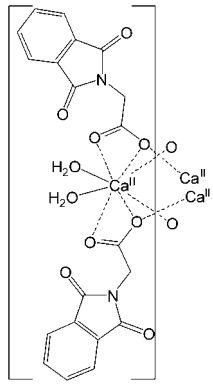
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.036; wR factor = 0.102; data-to-parameter ratio = 14.6.

In the title complex, $[Ca(C_{10}H_6NO_4)_2(H_2O)_2]_n$, the Ca^{II} atom lies on a twofold rotation axis and adopts a dodecahedral geometry. The Ca^{II} atom is octacoordinated by two O atoms from two water molecules and six O atoms from four acetate ligands. Each acetate acts as a tridentate ligand bridging two Ca^{II} atoms, resulting in a chain running along the c axis. O—H···O and C—H···O hydrogen bonds connect the chains into a two-dimensional network parallel to [011]. π–π interactions between adjacent isoindoline-1,3-dione rings [centroid–centroid distance = 3.4096 (11) Å] further consolidate the structure. One of the carboxylate O atoms is disordered over two sites in a 0.879 (12):0.121 (12) ratio.

Related literature

For background to *N*-phthaloylglycine, see: Khan & Ismail (2002). For related structures, see: Barooah *et al.* (2006).



Experimental

Crystal data

$[Ca(C_{10}H_6NO_4)_2(H_2O)_2]$
M_r = 484.43
Monoclinic, $C2/c$
a = 32.752 (1) Å
b = 9.0435 (3) Å
c = 6.9753 (3) Å
β = 99.020 (2)°
V = 2040.48 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 296 K
0.34 × 0.32 × 0.32 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*)
T_{min} = 0.884, T_{max} = 0.890
12481 measured reflections
2339 independent reflections
1847 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.102
S = 1.04
2339 reflections
160 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O4^{i}	0.82 (1)	2.10 (1)	2.907 (2)	171 (3)
O5—H5B···O4^{ii}	0.82 (1)	2.49 (2)	3.095 (2)	131 (2)
C8—H8···O2^{iii}	0.93	2.47	3.318 (2)	151

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008*b*); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

SS is grateful to the University of Hong Kong for providing facilities for crystallographic studies.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2422).

References

Barooah, N., Sarma, R. J., Batsanov, A. S. & Baruah, J. B. (2006). *Polyhedron*, **25**, 17–24.
Bruker. (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Khan, M. N. & Ismail, N. H. (2002). *J. Chem. Res.* **12**, 593–595.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *Mercury*. *J. Appl. Cryst*. **41**, 466-470.
Sheldrick, G. M. (2008*a*). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008*b*). *Acta Cryst.* A**64**, 112–122.

supporting information

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catena-Poly[[diaquacalcium]bis[μ-2-(1,3-dioxoisoindolin-2-yl)acetato]-$\kappa^3O,O':O;\kappa^3O:O,O'$]

Moazzam H. Bhatti, Uzma Yunus, Sohail Saeed, Syed Raza Shah and Wing-Tak Wong

S1. Comment

N-Phthaloylglycine is a simple *N*-phthaloylamino acid which has been widely studied for cleavage with various amines (Khan & Ismail, 2002) and metal complexation with interesting supramolecular structures (Barooah *et al.*, 2006). In an attempt to synthesis calcium(II) complex of N-phthaloylglycine, we have prepared a calcium complex of N-phthaloylglycine as the title compound and studied it crystal structure which is presented in this article.

In the title complex, the calcium ayom is octa-coordinated to two oxygen atoms from two water solvates and to 6 oxygen atoms from four acetate ligands. Each acetate acts as a tridentate ligand bridging two calcium centres resulting in a 1-D polymeric chain running along the *c*-axis. The calcium atom sits on a 2-fold axis, thus the asymmetric unit contains only half of the complex (Fig. 1).

The oxygen atom O1 is slightly disordered over two sites with occupancy factors 0.879 (12) and 0.121 (12). The acetate ring plane, C1/C2/O1/O2, makes a dihedral angle of 75.62 (8)° (77.0 (4)° for C1/C2/O1B/O2) with the ring plane of the isoindole-1,3-dione, N1/O3/O4/C3—C10.

There are inter-molecular O—H···O H-bonding interactions which link the molecules into a 2-D network parallel to the [0 1 1] plane (Fig. 2). There are also weak π–π interactions between adjacent isoindole-1,3-dione rings along the *c* axis in the crystal lattice; the distance between the centroids of the rings C4—C9 and (N1/C3/C4/C9/C10)* (*: x, 1 - y, 1/2 + z) being 3.4096 (11) Å. These π–π interactions help stacking the acetate ligand plane along the *c*-axis in the lattice.

S2. Experimental

The title compound was prepared from the reaction of $CaCl_2.2H_2O$ (0.01 mol) and sodium (1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl)acetate (0.02 mol) solution. Sodium (1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl)acetate was first obtained by adding 0.02 mol of (1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl)acetic acid to an aqueous solution of 0.02 mol $NaHCO_3$. The mixture was set aside to crystallize at ambient temperature for several days, giving suitable colorless single crystals.

S3. Refinement

All of the C-bound H atoms were observable from difference Fourier map but were placed at geometrical positions with C—H = 0.93 and 0.97 Å for phenyl and methylene H-atoms, respectively, and were refined using riding model with U_{iso}(H) = 1.2U_{eq}(C). The O-bound H-atoms were located from difference Fourier map and refined with bond distance restrains O–H = 0.82 (1) Å and H···H = 1.32 (1) Å with the thermal parameters set at U_{iso}(H) = 1.5U_{eq}(O). The oxygen atom O1 was disordered over two sites, with site occupancy factors 0.879 (12) and 0.121 (12).

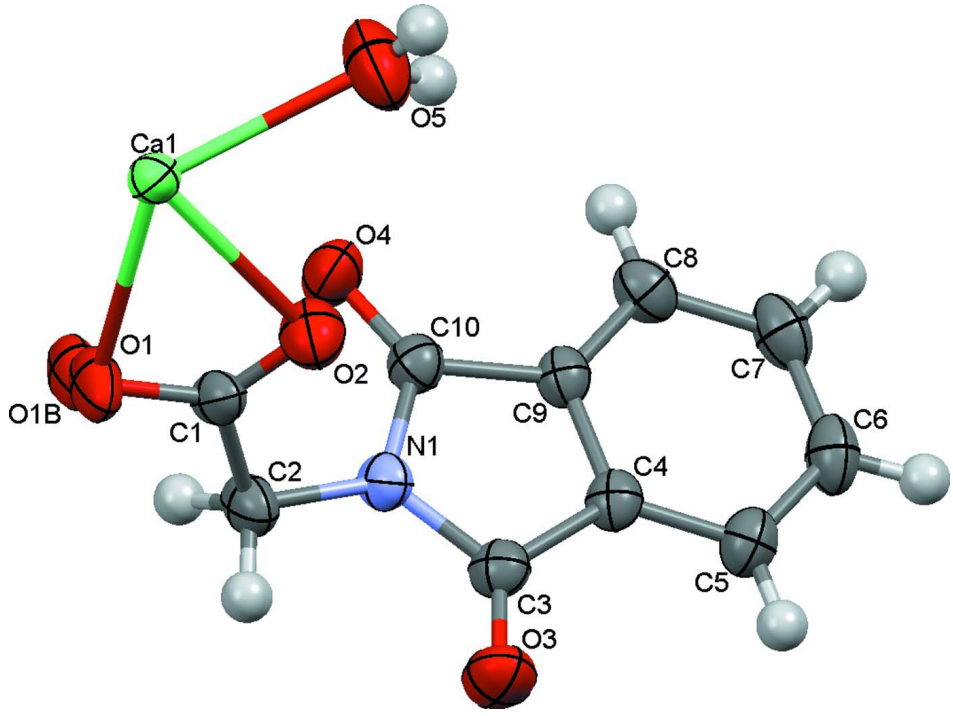

Figure 1

The asymmetric unit of the title complex drwan with 50% probability thermal ellipsoids showing the atom numbering scheme.

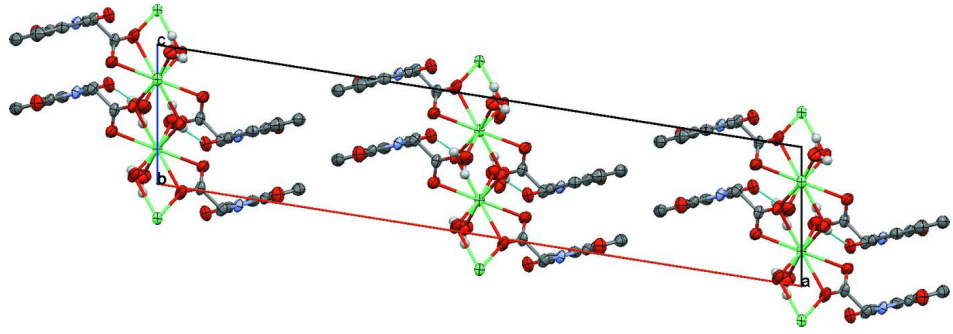

Figure 2

The packing diagram of the complex projected down the *b* axis showing the 1-D chain running parallel to the *c* axis; the cyan dotted lines indicate the H-bonding interactions.

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Crystal data

$[Ca(C_{10}H_6NO_4)_2(H_2O)_2]$
$M_r = 484.43$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 32.752$ (1) Å
$b = 9.0435$ (3) Å
$c = 6.9753$ (3) Å
$\beta = 99.020$ (2)°
$V = 2040.48$ (13) Å^3
$Z = 4$
$F(000) = 1000$
$D_x = 1.577$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 12481 reflections
$\theta = 2.3$–27.5°
$\mu = 0.37$ mm^{-1}

T = 296 K
Block, colourless

0.34 × 0.32 × 0.32 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*)
T_{min} = 0.884, T_{max} = 0.890

12481 measured reflections
2339 independent reflections
1847 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −42→42
k = −11→11
l = −8→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.102
S = 1.04
2339 reflections
160 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.9315P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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}	Occ. (<1)
Ca1	0.0000	0.12307 (5)	0.2500	0.02944 (16)	
O1	0.03670 (7)	0.0467 (4)	−0.0362 (7)	0.0520 (9)	0.879 (12)
O1B	0.0322 (5)	0.084 (2)	−0.126 (5)	0.0520 (9)	0.121 (12)
O2	0.07083 (4)	0.19128 (16)	0.1763 (2)	0.0468 (4)	
O3	0.18731 (4)	0.15606 (15)	0.0563 (2)	0.0509 (4)	
O4	0.07509 (4)	0.44337 (16)	−0.1576 (2)	0.0471 (4)	
O5	0.02298 (6)	0.3258 (2)	0.4645 (3)	0.0691 (5)	
H5A	0.0399 (7)	0.384 (3)	0.433 (4)	0.104*	
H5B	0.0228 (10)	0.337 (4)	0.5810 (11)	0.104*	
N1	0.12562 (4)	0.27067 (16)	−0.0647 (2)	0.0338 (3)	
C1	0.06666 (5)	0.12894 (18)	0.0183 (3)	0.0341 (4)	
C2	0.09973 (6)	0.1420 (2)	−0.1122 (3)	0.0387 (4)	
H2A	0.1168	0.0539	−0.0985	0.046*	

H2B	0.0865	0.1484	−0.2465	0.046*
C3	0.16724 (5)	0.2673 (2)	0.0189 (3)	0.0343 (4)
C4	0.17993 (5)	0.4252 (2)	0.0462 (3)	0.0320 (4)
C5	0.21772 (6)	0.4866 (2)	0.1170 (3)	0.0391 (4)
H5	0.2407	0.4280	0.1583	0.047*
C6	0.22000 (6)	0.6402 (2)	0.1243 (3)	0.0438 (5)
H6	0.2450	0.6852	0.1737	0.053*
C7	0.18598 (6)	0.7274 (2)	0.0598 (3)	0.0436 (5)
H7	0.1886	0.8298	0.0661	0.052*
C8	0.14793 (6)	0.6653 (2)	−0.0144 (3)	0.0380 (4)
H8	0.1251	0.7237	−0.0596	0.046*
C9	0.14567 (5)	0.5126 (2)	−0.0178 (2)	0.0311 (4)
C10	0.11039 (5)	0.41339 (19)	−0.0884 (3)	0.0331 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0250 (2)	0.0241 (2)	0.0391 (3)	0.000	0.00463 (19)	0.000
O1	0.0402 (9)	0.0575 (14)	0.062 (2)	−0.0247 (9)	0.0201 (11)	−0.0249 (15)
O1B	0.0402 (9)	0.0575 (14)	0.062 (2)	−0.0247 (9)	0.0201 (11)	−0.0249 (15)
O2	0.0444 (8)	0.0546 (9)	0.0438 (8)	−0.0091 (7)	0.0146 (6)	−0.0066 (7)
O3	0.0449 (8)	0.0355 (7)	0.0711 (11)	0.0061 (6)	0.0050 (7)	0.0046 (7)
O4	0.0340 (7)	0.0455 (8)	0.0583 (10)	−0.0011 (6)	−0.0033 (6)	0.0005 (7)
O5	0.0810 (13)	0.0671 (11)	0.0618 (11)	−0.0256 (9)	0.0189 (10)	−0.0254 (10)
N1	0.0300 (7)	0.0278 (7)	0.0450 (9)	−0.0056 (6)	0.0102 (6)	−0.0018 (6)
C1	0.0289 (8)	0.0235 (8)	0.0510 (12)	−0.0035 (6)	0.0093 (8)	−0.0023 (8)
C2	0.0388 (10)	0.0311 (9)	0.0486 (11)	−0.0100 (7)	0.0138 (8)	−0.0081 (8)
C3	0.0325 (9)	0.0339 (9)	0.0379 (10)	−0.0019 (7)	0.0102 (8)	0.0029 (8)
C4	0.0327 (9)	0.0353 (9)	0.0292 (9)	−0.0053 (7)	0.0082 (7)	0.0017 (7)
C5	0.0344 (9)	0.0444 (10)	0.0376 (10)	−0.0056 (8)	0.0033 (8)	0.0028 (9)
C6	0.0440 (11)	0.0475 (11)	0.0396 (11)	−0.0193 (9)	0.0052 (9)	−0.0022 (9)
C7	0.0582 (12)	0.0322 (9)	0.0413 (11)	−0.0149 (9)	0.0107 (10)	−0.0021 (8)
C8	0.0477 (11)	0.0311 (9)	0.0357 (10)	−0.0010 (8)	0.0076 (8)	0.0024 (8)
C9	0.0334 (9)	0.0322 (9)	0.0283 (9)	−0.0058 (7)	0.0069 (7)	0.0000 (7)
C10	0.0329 (9)	0.0326 (9)	0.0344 (10)	−0.0032 (7)	0.0072 (7)	0.0005 (7)

Geometric parameters (Å, º)

Ca1—O1B^{i}	2.258 (15)	O5—H5B	0.8199 (10)
Ca1—O1B^{ii}	2.258 (15)	N1—C10	1.384 (2)
Ca1—O1^{i}	2.338 (2)	N1—C3	1.396 (2)
Ca1—O1^{ii}	2.338 (2)	N1—C2	1.447 (2)
Ca1—O5	2.4111 (16)	C1—C2	1.525 (3)
Ca1—O5^{iii}	2.4111 (16)	C2—H2A	0.9700
Ca1—O2	2.5298 (13)	C2—H2B	0.9700
Ca1—O2^{iii}	2.5298 (13)	C3—C4	1.492 (2)
Ca1—O1^{iii}	2.581 (3)	C4—C5	1.375 (2)
Ca1—O1	2.581 (3)	C4—C9	1.388 (2)

Ca1—O1B	2.99 (3)	C5—C6	1.391 (3)
Ca1—O1B^{iii}	2.99 (3)	C5—H5	0.9300
O1—C1	1.242 (2)	C6—C7	1.382 (3)
O1—Ca1^{i}	2.338 (2)	C6—H6	0.9300
O1B—C1	1.45 (2)	C7—C8	1.391 (3)
O1B—Ca1^{i}	2.258 (15)	C7—H7	0.9300
O2—C1	1.226 (2)	C8—C9	1.383 (3)
O3—C3	1.207 (2)	C8—H8	0.9300
O4—C10	1.212 (2)	C9—C10	1.485 (2)
O5—H5A	0.8200 (10)		

O1B^{i}—Ca1—O1B^{ii}	67.6 (16)	O5—Ca1—O1B^{iii}	70.4 (6)
O1B^{i}—Ca1—O1^{i}	17.6 (8)	O5^{iii}—Ca1—O1B^{iii}	120.9 (3)
O1B^{ii}—Ca1—O1^{i}	82.0 (9)	O2—Ca1—O1B^{iii}	131.8 (5)
O1B^{i}—Ca1—O1^{ii}	82.0 (9)	O2^{iii}—Ca1—O1B^{iii}	52.5 (3)
O1B^{ii}—Ca1—O1^{ii}	17.6 (8)	O1^{iii}—Ca1—O1B^{iii}	11.8 (5)
O1^{i}—Ca1—O1^{ii}	97.9 (3)	O1—Ca1—O1B^{iii}	156.4 (4)
O1B^{i}—Ca1—O5	162.2 (7)	O1B—Ca1—O1B^{iii}	166.6 (9)
O1B^{ii}—Ca1—O5	108.2 (9)	C1—O1—Ca1^{i}	153.0 (2)
O1^{i}—Ca1—O5	167.07 (8)	C1—O1—Ca1	92.55 (18)
O1^{ii}—Ca1—O5	91.40 (14)	Ca1^{i}—O1—Ca1	114.46 (8)
O1B^{i}—Ca1—O5^{iii}	108.2 (9)	C1—O1B—Ca1^{i}	139.9 (19)
O1B^{ii}—Ca1—O5^{iii}	162.2 (7)	C1—O1B—Ca1	72.8 (11)
O1^{i}—Ca1—O5^{iii}	91.40 (14)	Ca1^{i}—O1B—Ca1	103.1 (9)
O1^{ii}—Ca1—O5^{iii}	167.07 (8)	C1—O2—Ca1	95.40 (11)
O5—Ca1—O5^{iii}	80.99 (11)	Ca1—O5—H5A	119 (2)
O1B^{i}—Ca1—O2	120.8 (5)	Ca1—O5—H5B	131 (2)
O1B^{ii}—Ca1—O2	83.9 (4)	H5A—O5—H5B	107 (3)
O1^{i}—Ca1—O2	115.25 (7)	C10—N1—C3	112.36 (14)
O1^{ii}—Ca1—O2	83.90 (6)	C10—N1—C2	122.35 (15)
O5—Ca1—O2	74.56 (6)	C3—N1—C2	125.20 (15)
O5^{iii}—Ca1—O2	84.00 (6)	O2—C1—O1	121.4 (2)
O1B^{i}—Ca1—O2^{iii}	83.9 (4)	O2—C1—O1B	135.8 (8)
O1B^{ii}—Ca1—O2^{iii}	120.8 (5)	O2—C1—C2	120.75 (15)
O1^{i}—Ca1—O2^{iii}	83.90 (6)	O1—C1—C2	117.7 (2)
O1^{ii}—Ca1—O2^{iii}	115.25 (7)	O1B—C1—C2	99.1 (10)
O5—Ca1—O2^{iii}	84.00 (6)	O2—C1—Ca1	59.82 (10)
O5^{iii}—Ca1—O2^{iii}	74.56 (6)	O1—C1—Ca1	62.24 (17)
O2—Ca1—O2^{iii}	151.77 (7)	O1B—C1—Ca1	78.9 (9)
O1B^{i}—Ca1—O1^{iii}	80.2 (6)	C2—C1—Ca1	175.44 (13)
O1B^{ii}—Ca1—O1^{iii}	74.1 (6)	N1—C2—C1	111.80 (15)
O1^{i}—Ca1—O1^{iii}	93.58 (5)	N1—C2—H2A	109.3
O1^{ii}—Ca1—O1^{iii}	65.54 (8)	C1—C2—H2A	109.3
O5—Ca1—O1^{iii}	82.03 (12)	N1—C2—H2B	109.3
O5^{iii}—Ca1—O1^{iii}	123.06 (6)	C1—C2—H2B	109.3
O2—Ca1—O1^{iii}	140.87 (9)	H2A—C2—H2B	107.9
O2^{iii}—Ca1—O1^{iii}	49.82 (5)	O3—C3—N1	124.85 (17)
O1B^{i}—Ca1—O1	74.1 (6)	O3—C3—C4	129.69 (17)

O1B^{ii}—Ca1—O1	80.2 (6)	N1—C3—C4	105.46 (14)
O1^{i}—Ca1—O1	65.54 (8)	C5—C4—C9	121.49 (17)
O1^{ii}—Ca1—O1	93.58 (5)	C5—C4—C3	130.51 (17)
O5—Ca1—O1	123.06 (6)	C9—C4—C3	107.99 (14)
O5^{iii}—Ca1—O1	82.03 (12)	C4—C5—C6	117.14 (18)
O2—Ca1—O1	49.82 (5)	C4—C5—H5	121.4
O2^{iii}—Ca1—O1	140.87 (9)	C6—C5—H5	121.4
O1^{iii}—Ca1—O1	148.96 (18)	C7—C6—C5	121.47 (17)
O1B^{i}—Ca1—O1B	76.9 (9)	C7—C6—H6	119.3
O1B^{ii}—Ca1—O1B	91.8 (5)	C5—C6—H6	119.3
O1^{i}—Ca1—O1B	65.2 (3)	C6—C7—C8	121.36 (18)
O1^{ii}—Ca1—O1B	105.4 (5)	C6—C7—H7	119.3
O5—Ca1—O1B	120.9 (3)	C8—C7—H7	119.3
O5^{iii}—Ca1—O1B	70.4 (6)	C9—C8—C7	116.88 (18)
O2—Ca1—O1B	52.5 (3)	C9—C8—H8	121.6
O2^{iii}—Ca1—O1B	131.8 (5)	C7—C8—H8	121.6
O1^{iii}—Ca1—O1B	156.4 (4)	C8—C9—C4	121.64 (16)
O1—Ca1—O1B	11.8 (5)	C8—C9—C10	130.22 (17)
O1B^{i}—Ca1—O1B^{iii}	91.8 (5)	C4—C9—C10	108.11 (15)
O1B^{ii}—Ca1—O1B^{iii}	76.9 (9)	O4—C10—N1	124.03 (16)
O1^{i}—Ca1—O1B^{iii}	105.4 (5)	O4—C10—C9	129.90 (17)
O1^{ii}—Ca1—O1B^{iii}	65.2 (3)	N1—C10—C9	106.06 (14)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O4^{iv}	0.82 (1)	2.10 (1)	2.907 (2)	171 (3)
O5—H5*B*···O4^{v}	0.82 (1)	2.49 (2)	3.095 (2)	131 (2)
C8—H8···O2^{vi}	0.93	2.47	3.318 (2)	151

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