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4,4′-(1,2-Diazaniumylethane-1,2-diyl)dibenzoate trihydrate

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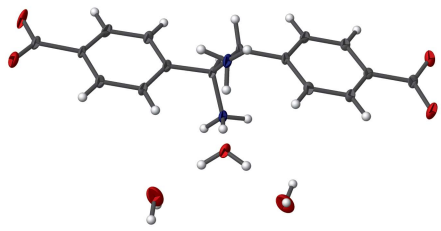
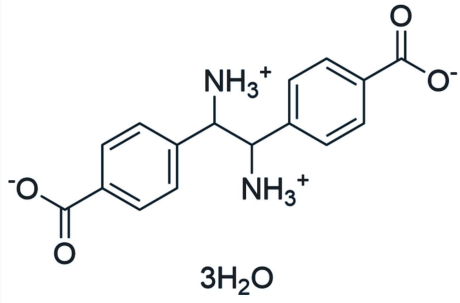
The title compound, $C_{16}H_{16}N_2O_4\cdot 3H_2O$, was synthesized from (1*R*,2*R*)-1,2-bis(2-hydroxyphenyl)ethylenediamine and terephthalaldehydic acid. The compound crystallizes from water as a double zwitterion with protonated amine groups and deprotonated carboxylate groups. The dihedral angle formed by the aromatic rings is 3.86 (11)°. In the crystal, N—H···O and O—H···O hydrogen bonds link molecules into a three-dimensional network.

3D view



Chemical scheme



Structure description

In recent years, dyes that led to an improvement in efficiency of the current generation of dye-sensitized solar cells (DSSC) have been devised (Nazeeruddin *et al.*, 1993; Hagfeldt *et al.*, 2010; Brewster *et al.*, 2013; Komatsu *et al.*, 2013; Brown *et al.*, 2013; Sinn *et al.*, 2014). In our laboratory, we have been engaged in the study of chiral salen-type complexes as dyes containing carboxyl groups which can be adsorbed on the surface of TiO_2, and with extended π-conjugated system in order to improve the power generation efficiency. During the course of this study, the title diamine compound as precursor of chiral salen-type ligands was synthesized, and its structure is reported herein. The molecule of the title compound crystallizes as a zwitterion with protonated amine groups NH_3^+ and deprotonated carboxylate groups COO^- (Fig. 1). The C—O bonds lengths within the carboxylate groups range from 1.252 (4) to 1.262 (3) Å, indicating delocalization of the negative charge, and are in good agreement with those observed in the organic zwitterion 4-(ammoniomethyl)benzoate (Atria *et al.*, 2014). The torsion angle C7—C8—C9—C10 is 178.8 (2)°. In the crystal, intermolecular N—H···O and O—H···O involving all ammonium groups, carboxylate groups and water molecules are observed, linking molecules into a three-dimensional network (Table 1).

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O5	0.91	2.01	2.911 (3)	173
N1—H1B···O3^{i}	0.91	1.80	2.686 (3)	165
N1—H1C···O2^{ii}	0.91	1.90	2.807 (3)	176
N2—H2A···O5	0.91	1.89	2.798 (3)	177
N2—H2B···O1^{iii}	0.91	1.93	2.787 (3)	156
N2—H2C···O6^{iv}	0.91	1.83	2.744 (4)	178
O7—H19···O1^{ii}	0.87 (5)	1.92 (5)	2.768 (4)	162 (5)
O7—H18···O2^{v}	0.89 (4)	1.81 (4)	2.688 (3)	166 (4)
O6—H20···O4^{vi}	0.87 (6)	1.85 (6)	2.720 (4)	172 (5)
O5—H17···O7	0.85 (7)	1.77 (7)	2.619 (4)	172 (6)
O6—H21···O3^{i}	0.81 (6)	1.93 (5)	2.696 (3)	157 (5)
O5—H16···O4^{vi}	0.84 (4)	1.83 (4)	2.654 (2)	166 (4)

Symmetry codes: (i) $x, y+1, z+1$; (ii) $x, y, z-1$; (iii) $x, y-1, z-1$; (iv) $x, y-1, z$; (v) $x+1, y, z-1$; (vi) $x+1, y+1, z+1$.

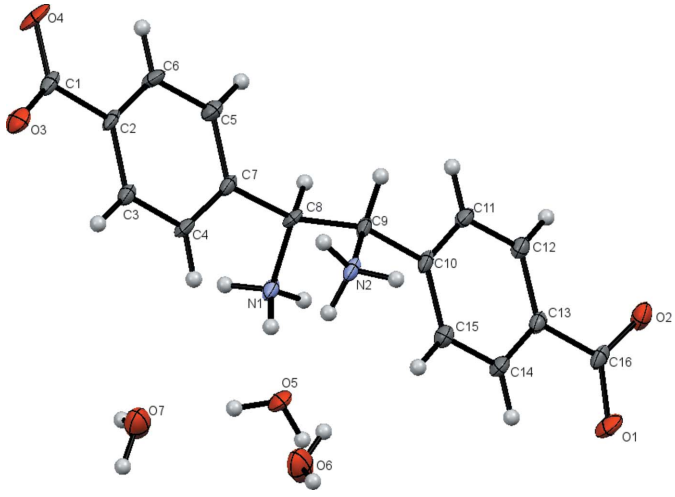


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

Synthesis and crystallization

To a solution of (1*R*,2*R*)-bis(2-hydroxyphenyl)ethylendiamine (1.222 g, 5 mmol) dissolved in ethanol (17 ml) was added 4-formylbenzoic acid (1.801 g, 12 mmol). The resulting mixture was stirred at 298 K for 3 h to give a yellow precipitate of (I), which was washed with water (5 ml), filtered off and dried in a vacuum. To a clear solution of (I) in tetrahydrofuran (THF, 50 ml) was added acidified water (HCl, 3.0 ml, 37%), and the mixture was stirred at 300 K for 3 h. The white precipitate afforded was filtered and washed with THF to give analytically pure 4,4′-(1,2-diazaniumylethane-1,2-diyl)dibenzoate (yield: 1.046 g, 69.7%). The compound was recrystallized by slow evaporation from a water solution to give colourless prismatic single crystals. IR (KBr, cm^{-1}): 421 (*w*), 505 (*w*), 540 (*w*), 606 (*w*), 667 (*w*), 743 (*w*), 777 (*w*), 863 (*w*), 977 (*w*), 1018 (*w*), 1078 (*w*), 1121 (*m*), 1181 (*m*), 1220 (*m*), 1384 (*m*), 1427 (*w*), 1469 (*m*), 1517 (*m*), 1572 (*m*), 1614 (*m*), 1697 (*s*, C═O), 2610 (*m*), 2976 (*s*), 3060 (*s*). MS (TOF–MASS) [M^-] calculated for $C_{16}H_{15}N_2O_4^-$ = 299.10; found = 299.13.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{16}N_2O_4{\cdot}3H_2O$
M_r	354.35
Crystal system, space group	Triclinic, *P*1
Temperature (K)	173
a, *b*, *c* (Å)	6.778 (3), 6.953 (3), 9.458 (4)
α, β, γ (°)	109.182 (6), 93.369 (6), 98.437 (6)
V (Å^3)	413.7 (3)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.49 × 0.34 × 0.07
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.946, 0.990
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2325, 2030, 1969
R_{int}	0.019
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.103, 1.03
No. of reflections	2030
No. of parameters	253
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.21
Absolute structure	Flack *x* determined using 217 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.2 (10)

Computer programs: *APEX2* (Bruker, 2013), *SAINT* (Bruker, 2013), *SHELXS2013* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The absolute configuration could not be determined unambigously as there was no significant anomalous dispersion using data collected with Mo radiation.

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full crystallographic data

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Crystal data

$C_{16}H_{16}N_2O_4·3H_2O$
M_r = 354.35
Triclinic, $P\overline{1}$
a = 6.778 (3) Å
b = 6.953 (3) Å
c = 9.458 (4) Å
α = 109.182 (6)°
β = 93.369 (6)°
γ = 98.437 (6)°
V = 413.7 (3) Å^3
Z = 1
$F(000)$ = 188
D_x = 1.422 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2325 reflections
θ = 2.3–27.5°
μ = 0.11 mm^{-1}
T = 173 K
Prism, colourless
0.49 × 0.34 × 0.07 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-forcus sealed tube
Detector resolution: 8.333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.946, T_{max} = 0.990
2325 measured reflections
2030 independent reflections
1969 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −8→8
k = −8→9
l = −12→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.03
2030 reflections
253 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0632P)^2 + 0.1469P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick 2015)
Extinction coefficient: 0.061 (11)
Absolute structure: Flack x determined using 217 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.2 (10)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C2	0.2668 (4)	−0.0431 (4)	0.0660 (3)	0.0148 (5)
C14	0.6379 (4)	0.5409 (4)	1.0399 (3)	0.0186 (6)
H14	0.7642	0.6159	1.0928	0.022*
C10	0.4424 (4)	0.3099 (4)	0.8089 (3)	0.0150 (5)
C13	0.4672 (4)	0.5516 (4)	1.1153 (3)	0.0154 (5)
C4	0.4811 (4)	0.1770 (4)	0.2925 (3)	0.0165 (5)
H4	0.6097	0.2517	0.3405	0.02*
C15	0.6259 (4)	0.4219 (4)	0.8886 (3)	0.0180 (5)
H15	0.7439	0.4169	0.8389	0.022*
C9	0.4215 (4)	0.1817 (4)	0.6422 (3)	0.0155 (5)
H9	0.3206	0.054	0.6262	0.019*
C1	0.2389 (4)	−0.1709 (4)	−0.1001 (3)	0.0177 (5)
C12	0.2827 (4)	0.4406 (4)	1.0366 (3)	0.0166 (5)
H12	0.1651	0.4459	1.0866	0.02*
C8	0.3387 (4)	0.2978 (4)	0.5438 (3)	0.0145 (5)
H8	0.2001	0.3148	0.5703	0.017*
C6	0.1036 (4)	−0.0325 (4)	0.1485 (3)	0.0189 (6)
H6	−0.0263	−0.1009	0.0992	0.023*
C5	0.1280 (4)	0.0772 (4)	0.3027 (3)	0.0188 (6)
H5	0.0154	0.0814	0.3582	0.023*
C3	0.4556 (4)	0.0630 (4)	0.1388 (3)	0.0156 (5)
H3	0.5681	0.0577	0.0831	0.019*
C16	0.4895 (4)	0.6773 (4)	1.2817 (3)	0.0167 (5)
C11	0.2706 (4)	0.3217 (4)	0.8846 (3)	0.0170 (5)
H11	0.1441	0.2476	0.8315	0.02*
C7	0.3178 (4)	0.1811 (4)	0.3758 (3)	0.0151 (5)
O4	0.0625 (3)	−0.2489 (3)	−0.1609 (2)	0.0281 (5)
O1	0.6571 (3)	0.7863 (3)	1.3418 (2)	0.0245 (5)
O3	0.3929 (3)	−0.1941 (3)	−0.1665 (2)	0.0240 (5)
O2	0.3413 (3)	0.6659 (3)	1.3551 (2)	0.0223 (4)
O6	0.7705 (4)	0.9702 (4)	0.8108 (3)	0.0346 (6)
O5	0.8755 (3)	0.4606 (3)	0.5889 (2)	0.0230 (4)
O7	0.9441 (4)	0.5415 (4)	0.3428 (3)	0.0338 (5)
N1	0.4571 (3)	0.5128 (3)	0.5815 (2)	0.0161 (4)
H1A	0.5904	0.5072	0.5822	0.024*
H1B	0.4329	0.5936	0.674	0.024*
H1C	0.4195	0.5676	0.5112	0.024*
N2	0.6159 (3)	0.1137 (3)	0.5979 (2)	0.0162 (4)
H2A	0.7043	0.2233	0.5941	0.024*

H2B	0.5935	0.0126	0.5057	0.024*
H2C	0.6677	0.064	0.6671	0.024*
H19	0.875 (7)	0.639 (7)	0.346 (5)	0.050 (13)*
H18	1.071 (6)	0.586 (5)	0.333 (4)	0.026 (9)*
H20	0.867 (8)	0.900 (8)	0.812 (6)	0.057 (14)*
H17	0.903 (8)	0.478 (8)	0.507 (7)	0.068 (16)*
H21	0.667 (8)	0.937 (8)	0.842 (6)	0.057 (15)*
H16	0.951 (6)	0.543 (7)	0.664 (5)	0.042 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0215 (12)	0.0117 (12)	0.0079 (11)	0.0007 (10)	−0.0062 (9)	0.0012 (9)
C14	0.0207 (13)	0.0203 (13)	0.0111 (12)	−0.0028 (10)	−0.0045 (9)	0.0044 (10)
C10	0.0225 (13)	0.0138 (12)	0.0079 (12)	0.0023 (10)	−0.0030 (9)	0.0036 (9)
C13	0.0209 (13)	0.0143 (12)	0.0112 (12)	0.0017 (10)	−0.0029 (9)	0.0058 (9)
C4	0.0168 (12)	0.0181 (13)	0.0102 (12)	−0.0016 (10)	−0.0060 (9)	0.0025 (9)
C15	0.0186 (13)	0.0217 (12)	0.0121 (12)	0.0000 (10)	−0.0009 (9)	0.0056 (10)
C9	0.0218 (12)	0.0165 (12)	0.0068 (11)	0.0016 (10)	−0.0028 (9)	0.0036 (9)
C1	0.0261 (14)	0.0130 (11)	0.0107 (12)	0.0028 (10)	−0.0067 (10)	0.0014 (9)
C12	0.0191 (13)	0.0184 (12)	0.0118 (12)	0.0012 (10)	−0.0018 (9)	0.0058 (10)
C8	0.0141 (11)	0.0162 (11)	0.0085 (11)	−0.0018 (9)	−0.0051 (8)	0.0012 (9)
C6	0.0157 (12)	0.0208 (13)	0.0146 (13)	−0.0025 (10)	−0.0078 (10)	0.0025 (10)
C5	0.0181 (13)	0.0213 (13)	0.0122 (12)	−0.0016 (10)	−0.0026 (10)	0.0023 (10)
C3	0.0176 (12)	0.0176 (12)	0.0102 (12)	0.0023 (10)	−0.0025 (9)	0.0040 (9)
C16	0.0226 (13)	0.0163 (12)	0.0116 (12)	0.0049 (10)	−0.0041 (9)	0.0056 (9)
C11	0.0189 (12)	0.0173 (12)	0.0119 (12)	−0.0012 (10)	−0.0053 (10)	0.0043 (10)
C7	0.0183 (12)	0.0156 (11)	0.0098 (12)	0.0019 (9)	−0.0049 (9)	0.0039 (9)
O4	0.0273 (10)	0.0318 (11)	0.0135 (10)	0.0040 (8)	−0.0128 (8)	−0.0049 (8)
O1	0.0239 (10)	0.0266 (10)	0.0143 (9)	0.0012 (8)	−0.0055 (7)	−0.0017 (8)
O3	0.0285 (10)	0.0241 (10)	0.0122 (9)	0.0006 (8)	−0.0014 (8)	−0.0010 (7)
O2	0.0245 (10)	0.0304 (10)	0.0128 (9)	0.0078 (8)	0.0013 (7)	0.0072 (7)
O6	0.0288 (12)	0.0487 (15)	0.0387 (13)	0.0121 (11)	0.0036 (10)	0.0291 (11)
O5	0.0235 (10)	0.0246 (10)	0.0129 (9)	−0.0058 (8)	−0.0052 (8)	0.0012 (8)
O7	0.0253 (12)	0.0523 (14)	0.0305 (12)	0.0073 (11)	0.0019 (9)	0.0229 (10)
N1	0.0210 (10)	0.0164 (10)	0.0089 (9)	0.0013 (8)	−0.0033 (8)	0.0034 (7)
N2	0.0227 (10)	0.0157 (9)	0.0086 (9)	0.0036 (8)	−0.0041 (7)	0.0030 (8)

Geometric parameters (Å, º)

C2—C6	1.387 (4)	C8—C7	1.516 (3)
C2—C3	1.393 (3)	C8—H8	1.0
C2—C1	1.514 (3)	C6—C5	1.393 (4)
C14—C13	1.393 (4)	C6—H6	0.95
C14—C15	1.389 (4)	C5—C7	1.396 (3)
C14—H14	0.95	C5—H5	0.95
C10—C15	1.394 (4)	C3—H3	0.95
C10—C11	1.401 (4)	C16—O1	1.255 (3)

C10—C9	1.521 (3)	C16—O2	1.262 (3)
C13—C12	1.394 (3)	C11—H11	0.95
C13—C16	1.514 (3)	O6—H20	0.88 (6)
C4—C7	1.394 (4)	O6—H21	0.81 (6)
C4—C3	1.395 (3)	O5—H17	0.85 (6)
C4—H4	0.95	O5—H16	0.83 (5)
C15—H15	0.95	O7—H19	0.87 (5)
C9—N2	1.501 (4)	O7—H18	0.89 (4)
C9—C8	1.549 (3)	N1—H1A	0.91
C9—H9	1.0	N1—H1B	0.91
C1—O4	1.256 (3)	N1—H1C	0.91
C1—O3	1.252 (4)	N2—H2A	0.91
C12—C11	1.394 (4)	N2—H2B	0.91
C12—H12	0.95	N2—H2C	0.91
C8—N1	1.507 (3)		

C6—C2—C3	119.0 (2)	C9—C8—H8	106.4
C6—C2—C1	120.1 (2)	C2—C6—C5	120.8 (2)
C3—C2—C1	120.9 (2)	C2—C6—H6	119.6
C13—C14—C15	120.9 (2)	C5—C6—H6	119.6
C13—C14—H14	119.5	C6—C5—C7	120.1 (2)
C15—C14—H14	119.5	C6—C5—H5	120.0
C15—C10—C11	118.5 (2)	C7—C5—H5	120.0
C15—C10—C9	122.3 (2)	C2—C3—C4	120.7 (2)
C11—C10—C9	119.1 (2)	C2—C3—H3	119.7
C14—C13—C12	119.0 (2)	C4—C3—H3	119.7
C14—C13—C16	118.8 (2)	O1—C16—O2	122.6 (2)
C12—C13—C16	122.1 (2)	O1—C16—C13	118.3 (2)
C7—C4—C3	120.0 (2)	O2—C16—C13	119.1 (2)
C7—C4—H4	120.0	C12—C11—C10	120.9 (2)
C3—C4—H4	120.0	C12—C11—H11	119.5
C14—C15—C10	120.6 (2)	C10—C11—H11	119.5
C14—C15—H15	119.7	C4—C7—C5	119.4 (2)
C10—C15—H15	119.7	C4—C7—C8	122.0 (2)
N2—C9—C10	110.8 (2)	C5—C7—C8	118.6 (2)
N2—C9—C8	112.81 (19)	H20—O6—H21	118 (5)
C10—C9—C8	111.31 (19)	H17—O5—H16	113 (4)
N2—C9—H9	107.2	H19—O7—H18	109 (4)
C10—C9—H9	107.2	C8—N1—H1A	109.5
C8—C9—H9	107.2	C8—N1—H1B	109.5
O4—C1—O3	124.7 (2)	H1A—N1—H1B	109.5
O4—C1—C2	117.4 (2)	C8—N1—H1C	109.5
O3—C1—C2	117.9 (2)	H1A—N1—H1C	109.5
C11—C12—C13	120.1 (2)	H1B—N1—H1C	109.5
C11—C12—H12	119.9	C9—N2—H2A	109.5
C13—C12—H12	119.9	C9—N2—H2B	109.5
N1—C8—C7	110.9 (2)	H2A—N2—H2B	109.5
N1—C8—C9	111.91 (18)	C9—N2—H2C	109.5

C7—C8—C9	114.34 (19)	H2A—N2—H2C	109.5
N1—C8—H8	106.4	H2B—N2—H2C	109.5
C7—C8—H8	106.4		
C15—C14—C13—C12	0.1 (4)	C1—C2—C6—C5	177.3 (2)
C15—C14—C13—C16	177.8 (2)	C2—C6—C5—C7	1.1 (4)
C13—C14—C15—C10	−0.2 (4)	C6—C2—C3—C4	0.5 (4)
C11—C10—C15—C14	0.6 (4)	C1—C2—C3—C4	−178.6 (2)
C9—C10—C15—C14	178.5 (2)	C7—C4—C3—C2	1.7 (4)
C15—C10—C9—N2	26.1 (3)	C14—C13—C16—O1	8.0 (4)
C11—C10—C9—N2	−155.9 (2)	C12—C13—C16—O1	−174.4 (2)
C15—C10—C9—C8	−100.3 (3)	C14—C13—C16—O2	−170.7 (2)
C11—C10—C9—C8	77.7 (3)	C12—C13—C16—O2	7.0 (4)
C6—C2—C1—O4	6.4 (4)	C13—C12—C11—C10	0.6 (4)
C3—C2—C1—O4	−174.5 (2)	C15—C10—C11—C12	−0.8 (4)
C6—C2—C1—O3	−172.6 (3)	C9—C10—C11—C12	−178.8 (2)
C3—C2—C1—O3	6.6 (4)	C3—C4—C7—C5	−2.5 (4)
C14—C13—C12—C11	−0.3 (4)	C3—C4—C7—C8	178.3 (2)
C16—C13—C12—C11	−177.9 (2)	C6—C5—C7—C4	1.2 (4)
N2—C9—C8—N1	−73.5 (2)	C6—C5—C7—C8	−179.6 (2)
C10—C9—C8—N1	51.7 (3)	N1—C8—C7—C4	47.4 (3)
N2—C9—C8—C7	53.6 (3)	C9—C8—C7—C4	−80.3 (3)
C10—C9—C8—C7	178.8 (2)	N1—C8—C7—C5	−131.8 (2)
C3—C2—C6—C5	−1.9 (4)	C9—C8—C7—C5	100.6 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O5	0.91	2.01	2.911 (3)	173
N1—H1*B*···O3^{i}	0.91	1.80	2.686 (3)	165
N1—H1*C*···O2^{ii}	0.91	1.90	2.807 (3)	176
N2—H2*A*···O5	0.91	1.89	2.798 (3)	177
N2—H2*B*···O1^{iii}	0.91	1.93	2.787 (3)	156
N2—H2*C*···O6^{iv}	0.91	1.83	2.744 (4)	178
O7—H19···O1^{ii}	0.87 (5)	1.92 (5)	2.768 (4)	162 (5)
O7—H18···O2^{v}	0.89 (4)	1.81 (4)	2.688 (3)	166 (4)
O6—H20···O4^{vi}	0.87 (6)	1.85 (6)	2.720 (4)	172 (5)
O5—H17···O7	0.85 (7)	1.77 (7)	2.619 (4)	172 (6)
O6—H21···O3^{i}	0.81 (6)	1.93 (5)	2.696 (3)	157 (5)
O5—H16···O4^{vi}	0.84 (4)	1.83 (4)	2.654 (2)	166 (4)

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