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Bis(dicyclohexylammonium 4-hydroxybenzoate)

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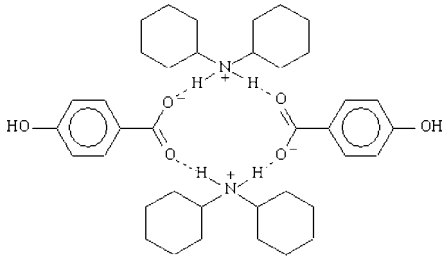
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.135; data-to-parameter ratio = 16.5.

In the crystal structure of the title compound, $2C_{12}H_{24}N^+\cdot 2C_7H_5O_3^-$, the cation is linked to the single-bonded carboxylate O atom of an anion as well as to the double-bonded carbonyl O atom of another anion to form a centrosymmetric hydrogen-bonded ion pair. Adjacent ion pairs are linked through the hydroxy group of the anion to produce a honeycomb-like layer structure.

Related literature

For crystal structures of dicyclohexylammonium salts of monocarboxylic acids, see Ng (1996, 1997, 1998), Ng *et al.* (1999, 2001), Ng & Hook (1999), Subramanian *et al.* (2000). For crystal structures of other ammonium salts of 4-hydroxybenzoic acid, see Moritani *et al.* (1987). For related literature, see: Aakeröy *et al.* (1993).



Experimental

Crystal data

$2C_{12}H_{24}N^+\cdot 2C_7H_5O_3^-$
M_r = 638.86
Monoclinic, $P2_1/n$
a = 9.4779 (2) Å
b = 11.0650 (3) Å
c = 17.5816 (4) Å
β = 95.431 (1)°
V = 1835.56 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 (2) K
0.35 × 0.30 × 0.06 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: none
32008 measured reflections
5346 independent reflections
4227 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.135
S = 1.04
5346 reflections
324 parameters
29 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1n···O1	0.87 (1)	1.96 (1)	2.808 (1)	164 (1)
N1—H2n···O2^{i}	0.86 (1)	1.85 (1)	2.706 (1)	169 (2)
O3—H3o···O1^{ii}	0.87 (1)	1.86 (1)	2.719 (1)	170 (2)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2167).

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supplementary materials

Acta Cryst. (2007). E**63**, o3303 [**doi:10.1107/S1600536807029856**]

Bis(dicyclohexylammonium 4-hydroxybenzoate)

S. M. Zain and S. W. Ng

Comment

4-Hydroxybenzoic acid is an excellent counterion for the engineering of ammonium salts that exhibit second-harmonic generation, as noted from the SHG activity of (*S*)-ethylphenylammonium 4-hydroxybenzoate (Aakeröy *et al.*, 1993). The anion is capable of mutiple hydrogen bonding interactions, this feature is crucial to chemical stability. We have previously used the sterically crowded dicyclohexylammonium cation in the synthesis of monocarboxylates (Ng, 1996; Ng, 1997; Ng, 1998; Ng & Hook, 1999; Ng *et al.*, 1999, 2001; Subramanian *et al.*, 2000) but these monocarboxylates do not have hydrogen-bond donor sites. Our studies are now extended to a study of dicyclohexylammonium 4-hydroxybenzoate, which exists as a hydrogen-bonded dimeric ion-pair that is linked across a center-of-inversion (Fig. 1). The ammonium hydrogen serves as as donor to a single-bond carboxyl oxygen atom of one anion as well as to the double-bond carbonyl oxygen atom of the symmetry-related anion. The carboxylate $–CO_2$ unit has localized bonds: the hydrogen bond to the negatively-charged oxygen atom is significantly longer than that to the neutral oxygen atom. The hydroxy group engages in linking adjacent dimeric ion-pairs into a layer motif (Table 1, Fig. 2). The layer has a honeycomb-like topology (Fig. 3) but is buckled.

The crystal structures of polymethyleneiminium 4-hydroxybenzoates, $[(CH_2)_nNH_2]$ $[C_7H_5O_3]$ (n = 4, 5 and 6) have been reported; the hexamethyleneiminiums exists in two modifications (Moritani *et al.*, 1987). The compounds, whose carboxylate groups are also localized, adopt chain motif instead, a motif that is also adopted by dicyclohexylammonium trifluoroacetate (Ng *et al.*, 1999).

Experimental

Dicyclohexylamine (0.17 g, 1 mmol) and 4-hydroxybenzoic acid (0.14 g, 1 mmol) were dissolved in ethanol (25 ml). The mixture was heated to dissolve the reactants. Colorless plates of the salt separated from the solution after several days.

Refinement

All hydrogen atoms were located in difference Fourier maps, and were refined with distance restraints C–H = 0.95±0.01 Å and N–H = O–H = 0.85±0.01 Å. The temperature factors were refined freely.

Figures

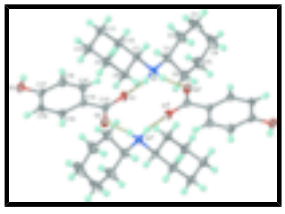

Fig. 1. **Figure 1**. Thermal ellipsoid plot of the hydrogen-bonded dimer; displacement ellipsoids are drawn at the 70% probability level. The dashed lines denote hydrogen bonds. [Symmetry code *i*: 1 – *x*, 1 – *y*, 1 – *z*.]

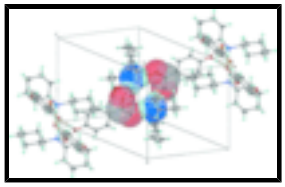

Fig. 2. **Figure 2**. Layer structure; displacement ellipsoids are drawn at the 70% probability level. The dashed lines denote hydrogen bonds, and the atoms constituting the 12-membered O–C=O···H–N–H···O–C=O···H–N–H··· ring are shown with their van der Waals surfaces.

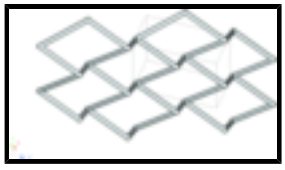

Fig. 3. **Figure 3**. *OLEX* depiction of the (6,3)-honeycomb topology, shown projected against the unit cell.

(I)

Crystal data

$2C_{12}H_{24}N^{+}\cdot 2C_7H_5O_3^{-}$	$F_{000} = 696$
$M_r = 638.86$	$D_x = 1.156$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 9647 reflections
$a = 9.4779$ (2) Å	$\theta = 2.4$–34.6°
$b = 11.0650$ (3) Å	$\mu = 0.08$ mm^{-1}
$c = 17.5816$ (4) Å	$T = 173$ (2) K
$\beta = 95.431$ (1)°	Plate, colorless
$V = 1835.56$ (8) Å^3	0.35 × 0.30 × 0.06 mm
$Z = 2$	

Data collection

Bruker APEX2 area-detector diffractometer	4227 reflections with $I > 2\sigma(I)$
Radiation source: medium-focus sealed tube	$R_{int} = 0.033$
Monochromator: graphite	$\theta_{max} = 30.0^{\circ}$
$T = 173(2)$ K	$\theta_{min} = 2.6^{\circ}$
φ and ω scans	$h = -13\rightarrow13$
Absorption correction: none	$k = -15\rightarrow15$
32008 measured reflections	$l = -24\rightarrow24$
5346 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	All H-atom parameters refined
$wR(F^2) = 0.135$	$w = 1/[\sigma^2(F_o^2) + (0.0739P)^2 + 0.5355P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
5346 reflections	$\Delta\rho_{max}$ = 0.52 e Å^{-3}
324 parameters	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
29 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.3950 (1)	0.6161 (1)	0.3722 (1)	0.0201 (2)
O2	0.2552 (1)	0.6278 (1)	0.4673 (1)	0.0238 (2)
O3	0.0294 (1)	1.0816 (1)	0.2716 (1)	0.0224 (2)
N1	0.6664 (1)	0.5639 (1)	0.4429 (1)	0.0159 (2)
C1	0.7400 (1)	0.5365 (1)	0.3728 (1)	0.0193 (2)
C2	0.9009 (1)	0.5378 (2)	0.3891 (1)	0.0312 (3)
C3	0.9688 (2)	0.5083 (2)	0.3159 (1)	0.0472 (5)
C4	0.9177 (2)	0.3876 (2)	0.2818 (1)	0.0439 (4)
C5	0.7560 (1)	0.3837 (1)	0.2691 (1)	0.0305 (3)
C6	0.6884 (1)	0.4135 (1)	0.3423 (1)	0.0224 (2)
C7	0.7084 (1)	0.6764 (1)	0.4870 (1)	0.0163 (2)
C8	0.6200 (1)	0.6816 (1)	0.5551 (1)	0.0185 (2)
C9	0.6546 (1)	0.7949 (1)	0.6030 (1)	0.0210 (2)
C10	0.6305 (1)	0.9076 (1)	0.5536 (1)	0.0222 (2)
C11	0.7201 (1)	0.9028 (1)	0.4858 (1)	0.0227 (2)
C12	0.6889 (1)	0.7891 (1)	0.4374 (1)	0.0201 (2)
C13	0.2947 (1)	0.6642 (1)	0.4052 (1)	0.0165 (2)
C14	0.2207 (1)	0.7721 (1)	0.3683 (1)	0.0152 (2)
C15	0.2559 (1)	0.8142 (1)	0.2979 (1)	0.0182 (2)
C16	0.1924 (1)	0.9166 (1)	0.2646 (1)	0.0194 (2)
C17	0.0917 (1)	0.9792 (1)	0.3017 (1)	0.0178 (2)
C18	0.0528 (1)	0.9369 (1)	0.3717 (1)	0.0190 (2)
C19	0.1173 (1)	0.8343 (1)	0.4046 (1)	0.0176 (2)
H3o	0.063 (2)	1.096 (2)	0.228 (1)	0.052 (6)*
H1n	0.577 (1)	0.571 (1)	0.428 (1)	0.019 (3)*
H2n	0.680 (2)	0.503 (1)	0.473 (1)	0.036 (4)*
H1	0.709 (2)	0.597 (1)	0.337 (1)	0.022 (4)*
H21	0.929 (2)	0.481 (1)	0.429 (1)	0.036 (4)*
H22	0.933 (2)	0.615 (1)	0.409 (1)	0.038 (5)*
H31	1.069 (1)	0.507 (2)	0.327 (1)	0.061 (6)*
H32	0.949 (3)	0.570 (2)	0.278 (1)	0.077 (8)*
H41	0.946 (2)	0.323 (1)	0.318 (1)	0.049 (6)*
H42	0.959 (2)	0.372 (2)	0.235 (1)	0.054 (6)*
H51	0.727 (2)	0.304 (1)	0.253 (1)	0.044 (5)*
H52	0.728 (2)	0.445 (1)	0.232 (1)	0.029 (4)*
H61	0.587 (1)	0.414 (1)	0.334 (1)	0.024 (4)*
H62	0.713 (2)	0.355 (1)	0.381 (1)	0.034 (4)*
H7	0.807 (1)	0.667 (1)	0.505 (1)	0.020 (3)*

H81	0.635 (2)	0.610 (1)	0.585 (1)	0.023 (4)*
H82	0.522 (1)	0.685 (2)	0.536 (1)	0.030 (4)*
H91	0.753 (1)	0.795 (1)	0.625 (1)	0.026 (4)*
H92	0.595 (1)	0.796 (1)	0.645 (1)	0.024 (4)*
H101	0.651 (2)	0.979 (1)	0.583 (1)	0.028 (4)*
H102	0.532 (1)	0.911 (1)	0.533 (1)	0.022 (4)*
H111	0.818 (1)	0.906 (1)	0.506 (1)	0.026 (4)*
H112	0.706 (2)	0.975 (1)	0.455 (1)	0.028 (4)*
H121	0.594 (1)	0.790 (1)	0.413 (1)	0.024 (4)*
H122	0.751 (1)	0.787 (2)	0.398 (1)	0.028 (4)*
H15	0.324 (1)	0.769 (1)	0.272 (1)	0.026 (4)*
H16	0.218 (2)	0.947 (2)	0.217 (1)	0.028 (4)*
H18	−0.017 (1)	0.981 (1)	0.395 (1)	0.029 (4)*
H19	0.096 (2)	0.807 (1)	0.453 (1)	0.026 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0204 (4)	0.0178 (4)	0.0214 (4)	0.0044 (3)	−0.0021 (3)	−0.0041 (3)
O2	0.0307 (4)	0.0195 (4)	0.0211 (4)	0.0056 (3)	0.0024 (3)	0.0052 (3)
O3	0.0265 (4)	0.0160 (4)	0.0247 (4)	0.0036 (3)	0.0019 (3)	0.0053 (3)
N1	0.0173 (4)	0.0147 (4)	0.0156 (4)	0.0007 (3)	0.0007 (3)	−0.0009 (3)
C1	0.0183 (5)	0.0226 (5)	0.0172 (5)	0.0011 (4)	0.0027 (4)	−0.0052 (4)
C2	0.0187 (5)	0.0415 (8)	0.0334 (7)	−0.0008 (5)	0.0019 (5)	−0.0174 (6)
C3	0.0210 (6)	0.0725 (13)	0.0499 (9)	−0.0063 (7)	0.0127 (6)	−0.0310 (9)
C4	0.0272 (7)	0.0609 (11)	0.0439 (9)	0.0101 (7)	0.0050 (6)	−0.0269 (8)
C5	0.0275 (6)	0.0362 (7)	0.0280 (6)	0.0029 (5)	0.0029 (5)	−0.0136 (6)
C6	0.0225 (5)	0.0226 (6)	0.0216 (5)	0.0022 (4)	0.0001 (4)	−0.0066 (4)
C7	0.0191 (5)	0.0139 (5)	0.0157 (5)	−0.0006 (4)	−0.0001 (4)	−0.0019 (4)
C8	0.0255 (5)	0.0151 (5)	0.0148 (5)	0.0004 (4)	0.0020 (4)	0.0001 (4)
C9	0.0287 (6)	0.0180 (5)	0.0163 (5)	0.0008 (4)	0.0014 (4)	−0.0020 (4)
C10	0.0284 (6)	0.0148 (5)	0.0234 (5)	0.0006 (4)	0.0037 (4)	−0.0017 (4)
C11	0.0290 (6)	0.0153 (5)	0.0242 (6)	−0.0032 (4)	0.0049 (4)	0.0005 (4)
C12	0.0262 (5)	0.0171 (5)	0.0170 (5)	−0.0025 (4)	0.0028 (4)	0.0017 (4)
C13	0.0177 (5)	0.0127 (5)	0.0182 (5)	−0.0005 (4)	−0.0030 (4)	−0.0019 (4)
C14	0.0154 (4)	0.0128 (5)	0.0169 (5)	−0.0005 (4)	−0.0005 (3)	−0.0002 (4)
C15	0.0182 (5)	0.0187 (5)	0.0177 (5)	0.0004 (4)	0.0025 (4)	−0.0010 (4)
C16	0.0216 (5)	0.0201 (5)	0.0166 (5)	−0.0007 (4)	0.0017 (4)	0.0027 (4)
C17	0.0187 (5)	0.0136 (5)	0.0204 (5)	−0.0015 (4)	−0.0019 (4)	0.0013 (4)
C18	0.0188 (5)	0.0160 (5)	0.0227 (5)	0.0018 (4)	0.0045 (4)	−0.0005 (4)
C19	0.0190 (5)	0.0161 (5)	0.0179 (5)	−0.0007 (4)	0.0035 (4)	0.0013 (4)

Geometric parameters (Å, °)

O1—C13	1.276 (1)	C1—H1	0.95 (1)
O2—C13	1.254 (1)	C2—H21	0.96 (1)
O3—C17	1.362 (1)	C2—H22	0.96 (1)
N1—C1	1.503 (1)	C3—H31	0.95 (1)
N1—C7	1.501 (1)	C3—H32	0.96 (1)

C1—C2	1.525 (2)	C4—H41	0.97 (1)
C1—C6	1.526 (2)	C4—H42	0.96 (1)
C2—C3	1.528 (2)	C5—H51	0.96 (1)
C3—C4	1.524 (2)	C5—H52	0.96 (1)
C4—C5	1.529 (2)	C6—H61	0.96 (1)
C5—C6	1.528 (2)	C6—H62	0.95 (1)
C7—C12	1.523 (2)	C7—H7	0.96 (1)
C7—C8	1.526 (2)	C9—H91	0.97 (1)
C9—C10	1.525 (2)	C9—H92	0.97 (1)
C9—C8	1.528 (2)	C10—H101	0.96 (1)
C10—C11	1.528 (2)	C10—H102	0.97 (1)
C11—C12	1.532 (2)	C11—H111	0.96 (1)
C13—C14	1.500 (2)	C11—H112	0.97 (1)
C14—C15	1.393 (2)	C8—H81	0.95 (1)
C14—C19	1.399 (2)	C8—H82	0.96 (1)
C15—C16	1.386 (2)	C12—H121	0.96 (1)
C16—C17	1.390 (2)	C12—H122	0.96 (1)
C17—C18	1.399 (2)	C15—H15	0.97 (1)
C18—C19	1.390 (2)	C16—H16	0.96 (1)
O3—H3o	0.87 (1)	C18—H18	0.95 (1)
N1—H1n	0.87 (1)	C19—H19	0.95 (1)
N1—H2n	0.86 (1)		
C1—N1—C7	118.0 (1)	C5—C4—H41	107 (1)
N1—C1—C2	112.2 (1)	C3—C4—H42	111 (1)
N1—C1—C6	108.0 (1)	C5—C4—H42	111 (1)
C2—C1—C6	110.9 (1)	H41—C4—H42	108 (2)
C1—C2—C3	109.5 (1)	C6—C5—H51	108 (1)
C4—C3—C2	112.0 (2)	C4—C5—H51	109 (1)
C3—C4—C5	111.1 (1)	C6—C5—H52	108 (1)
C6—C5—C4	111.4 (1)	C4—C5—H52	107 (1)
C1—C6—C5	110.1 (1)	H51—C5—H52	114 (2)
N1—C7—C12	111.8 (1)	C1—C6—H61	110 (1)
N1—C7—C8	107.4 (1)	C5—C6—H61	111 (1)
C12—C7—C8	111.9 (1)	C1—C6—H62	108 (1)
C10—C9—C8	110.2 (1)	C5—C6—H62	111 (1)
C9—C10—C11	110.6 (1)	H61—C6—H62	107 (1)
C10—C11—C12	111.6 (1)	N1—C7—H7	106 (1)
C7—C8—C9	111.0 (1)	C12—C7—H7	110 (1)
C7—C12—C11	110.4 (1)	C8—C7—H7	110 (1)
O1—C13—O2	124.0 (1)	C10—C9—H91	108 (1)
O2—C13—C14	117.7 (1)	C8—C9—H91	111 (1)
O1—C13—C14	118.3 (1)	C10—C9—H92	111 (1)
C15—C14—C19	118.5 (1)	C8—C9—H92	109 (1)
C15—C14—C13	120.6 (1)	H91—C9—H92	108 (1)
C19—C14—C13	120.9 (1)	C9—C10—H101	111 (1)
C16—C15—C14	121.2 (1)	C11—C10—H101	111 (1)
C15—C16—C17	119.9 (1)	C9—C10—H102	109 (1)
O3—C17—C16	121.6 (1)	C11—C10—H102	107 (1)
O3—C17—C18	118.6 (1)	H101—C10—H102	108 (1)

C16—C17—C18	119.7 (1)	C10—C11—H111	108 (1)
C19—C18—C17	119.9 (1)	C12—C11—H111	111 (1)
C18—C19—C14	120.8 (1)	C10—C11—H112	110 (1)
C17—O3—H3o	108 (1)	C12—C11—H112	111 (1)
C7—N1—H1n	107 (1)	H111—C11—H112	105 (1)
C1—N1—H1n	106 (1)	C7—C8—H81	109 (1)
C7—N1—H2n	108 (1)	C9—C8—H81	112 (1)
C1—N1—H2n	107 (1)	C7—C8—H82	109 (1)
H1n—N1—H2n	110 (2)	C9—C8—H82	108 (1)
N1—C1—H1	106 (1)	H81—C8—H82	108 (1)
C2—C1—H1	111 (1)	C7—C12—H121	109 (1)
C6—C1—H1	109 (1)	C11—C12—H121	111 (1)
C1—C2—H21	110 (1)	C7—C12—H122	111 (1)
C3—C2—H21	111 (1)	C11—C12—H122	109 (1)
C1—C2—H22	110 (1)	H121—C12—H122	107 (1)
C3—C2—H22	110 (1)	C16—C15—H15	120 (1)
H21—C2—H22	106 (2)	C14—C15—H15	119 (1)
C4—C3—H31	110 (1)	C15—C16—H16	121 (1)
C2—C3—H31	109 (1)	C17—C16—H16	119 (1)
C4—C3—H32	108 (2)	C19—C18—H18	122 (1)
C2—C3—H32	112 (2)	C17—C18—H18	118 (1)
H31—C3—H32	106 (2)	C18—C19—H19	121 (1)
C3—C4—H41	109 (1)	C14—C19—H19	119 (1)
C7—N1—C1—C2	52.8 (1)	N1—C7—C12—C11	175.0 (1)
C7—N1—C1—C6	175.3 (1)	C8—C7—C12—C11	54.5 (1)
N1—C1—C2—C3	179.5 (1)	C10—C11—C12—C7	−55.0 (1)
C6—C1—C2—C3	58.7 (2)	O2—C13—C14—C15	−177.6 (1)
C1—C2—C3—C4	−56.6 (2)	O1—C13—C14—C15	3.4 (2)
C2—C3—C4—C5	54.6 (2)	O2—C13—C14—C19	3.9 (2)
C3—C4—C5—C6	−54.1 (2)	O1—C13—C14—C19	−175.1 (1)
N1—C1—C6—C5	177.8 (1)	C19—C14—C15—C16	1.1 (2)
C2—C1—C6—C5	−58.9 (1)	C13—C14—C15—C16	−177.4 (1)
C4—C5—C6—C1	56.3 (2)	C14—C15—C16—C17	0.0 (2)
C1—N1—C7—C12	57.7 (1)	C15—C16—C17—O3	178.5 (1)
C1—N1—C7—C8	−179.2 (1)	C15—C16—C17—C18	−1.3 (2)
C8—C9—C10—C11	−57.5 (1)	O3—C17—C18—C19	−178.4 (1)
C9—C10—C11—C12	57.0 (1)	C16—C17—C18—C19	1.5 (2)
N1—C7—C8—C9	−179.3 (1)	C17—C18—C19—C14	−0.4 (2)
C12—C7—C8—C9	−56.2 (1)	C15—C14—C19—C18	−1.0 (2)
C10—C9—C8—C7	57.1 (1)	C13—C14—C19—C18	177.6 (1)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*n*···O1	0.87 (1)	1.96 (1)	2.808 (1)	164 (1)
N1—H2*n*···O2^{i}	0.86 (1)	1.85 (1)	2.706 (1)	169 (2)
O3—H3*o*···O1^{ii}	0.87 (1)	1.86 (1)	2.719 (1)	170 (2)

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

Fig. 1

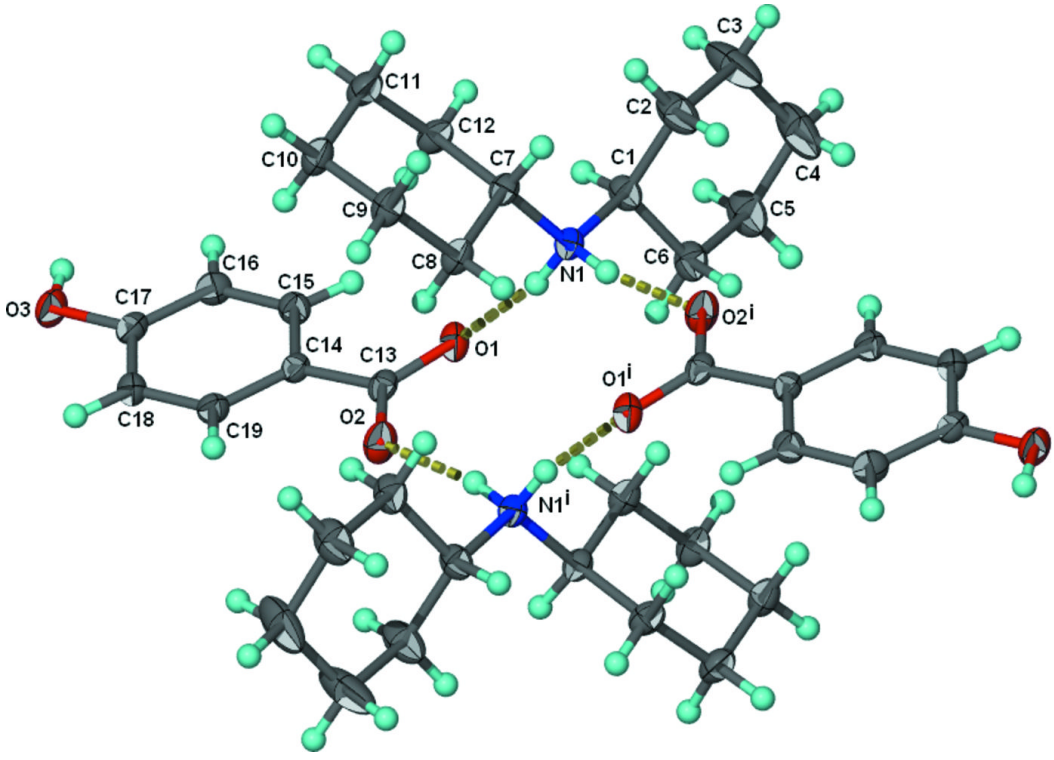
C3
C11
C2
C12
C10
C7
C1
C4
C9
C5
C8
N1
C6
C16
C15
O3
C17
O2i
C14
C13
O1
O1i
C18
C19
O2
N1i

Fig. 2

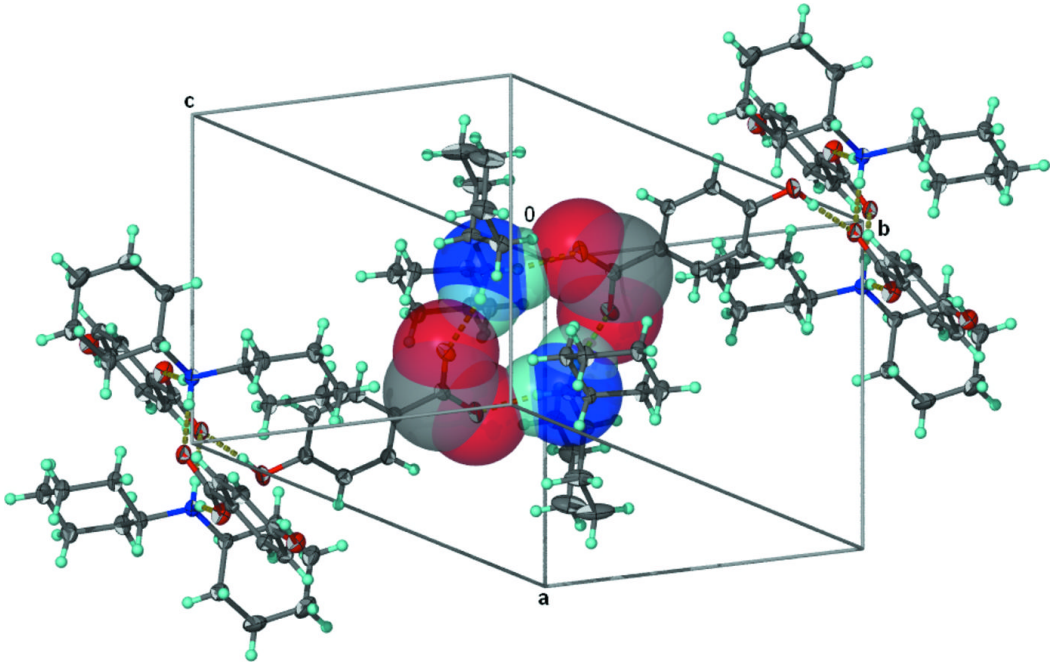

Fig. 3