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Dimethylammonium 4-hydroxybenzoate

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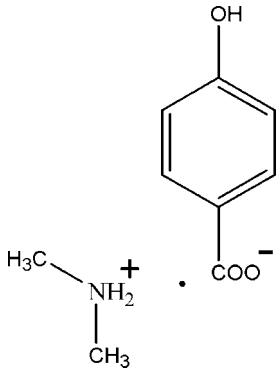
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.143; data-to-parameter ratio = 19.6.

In the crystal structure of the title compound, $C_2H_8N^+\cdot C_7H_5O_3^-$, the anions and cations are linked by O—H···O and N—H···O hydrogen bonds into layers parallel to the *ac* plane.

Related literature

For related structures, see: Hemamalini *et al.* (2011). Chitradevi *et al.* (2009).



Experimental

Crystal data

$C_2H_8N^+\cdot C_7H_5O_3^-$
M_r = 183.20
Orthorhombic, *Pbca*
a = 10.2980 (8) Å
b = 10.0586 (9) Å
c = 19.2595 (17) Å
V = 1995.0 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.18 × 0.16 × 0.14 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.984, T_{max} = 0.987
9496 measured reflections
2394 independent reflections
1673 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.143
S = 1.04
2394 reflections
122 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O3	0.90	1.87	2.7614 (18)	169
O1—H1···O2^{i}	0.82	1.81	2.6183 (17)	171
N1—H1B···O2^{ii}	0.90	1.82	2.7131 (17)	170

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

The authors wish to acknowledge the SAIF, IIT, Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5869).

References

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Hemamalini, M., Goh, J. H. & Fun, H.-K. (2011). *Acta Cryst.* E**67**, o3121.
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supporting information

Acta Cryst. (2012). E**68**, o1445 [doi:10.1107/S1600536812016145]

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S1. Comment

The goemetric parameters of the title compound (Fig. 1) are comparable with those in related structures (Hemamalini *et al.*, 2011; Chitradevi *et al.*, 2009).

The molecular structure is stabilized by intramolecular N—H···O hydrogen bond and the crystal structure is formed by weak intermolecular O—H···O and N-H···O (Fig. 2 & Table 1) interactions.

S2. Experimental

A solution of *p*-hydroxybenzoic acid (0.138g, 1 mmol) in 10 ml ethanol was added with stirring to a solution of dimethylamine (0.450g, 1 mmol) in 10 ml of distilled water at 303 K. After some time, a white precipitate was obtained. The white precipitate was dissolved in ethanol and colourless single crystals suitable for X-ray diffraction were obtained by slow evaporation of the ethanol solution.

S3. Refinement

All H atoms were located in a difference map, but positioned geometrically with O—H = 0.82Å, N—H = 0.90Å and C—H = 0.93–0.97 Å and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(C_{methyl},O).

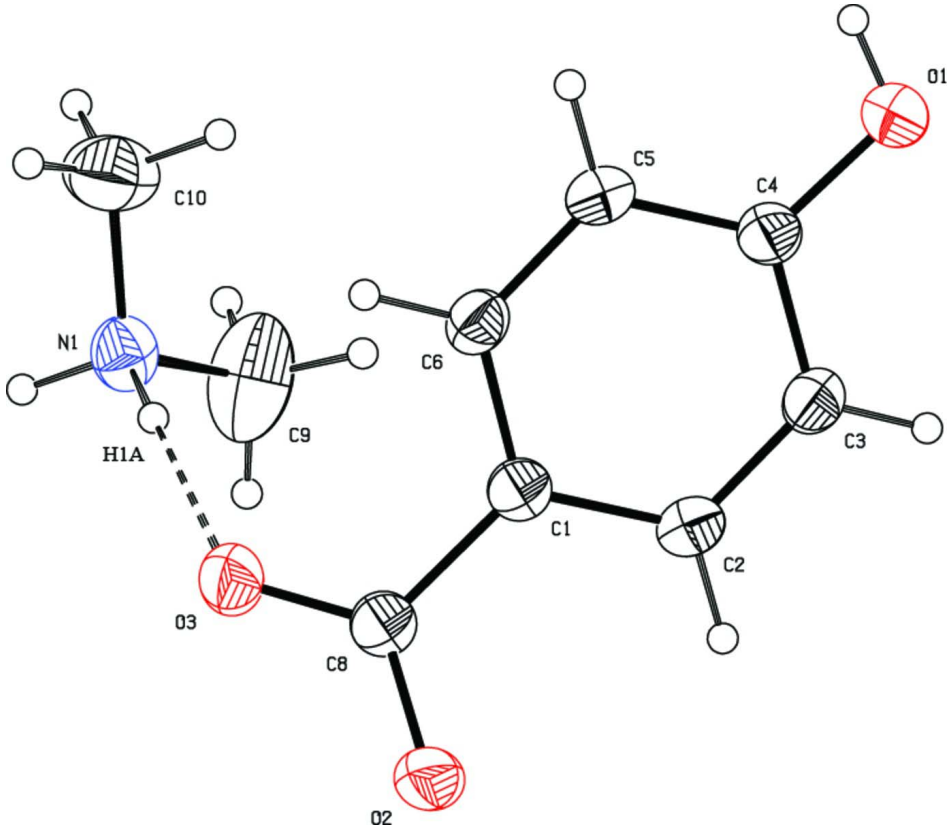

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

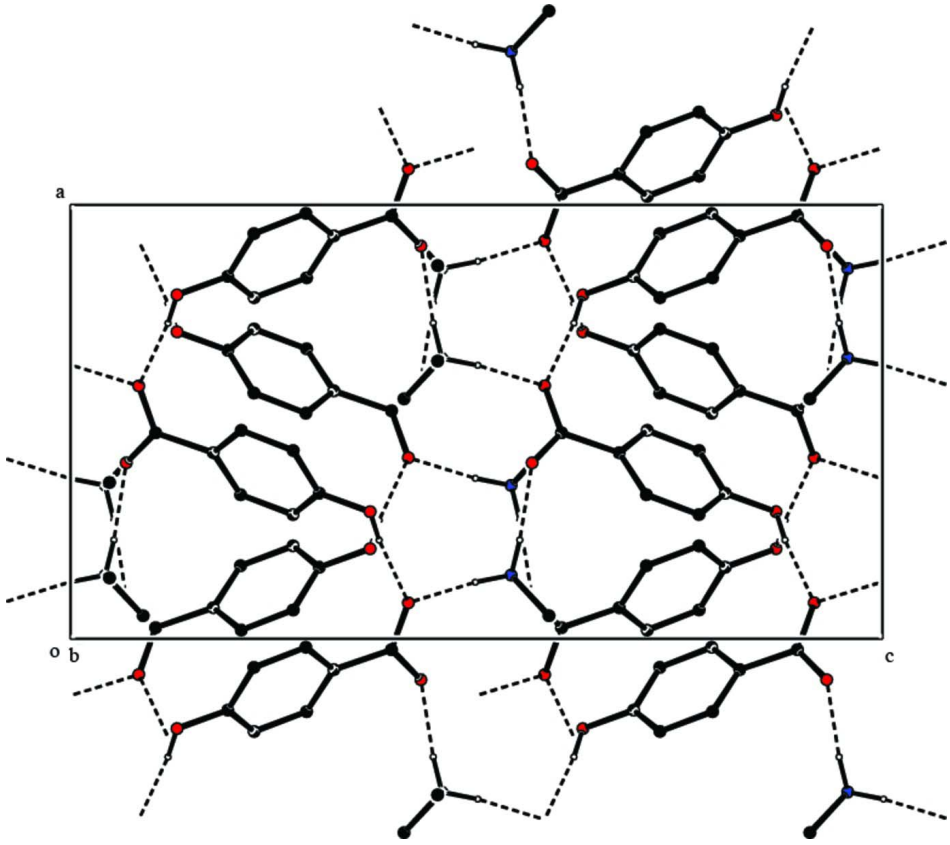

Figure 2

The packing of (I), viewed down *b* axis. Intermolecular Hydrogen bond is shown as dashed line. H atoms not involved in hydrogen bonding have been omitted.

Dimethylammonium 4-hydroxybenzoate

Crystal data

$C_2H_8N^+·C_7H_5O_3^-$
M_r = 183.20
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 10.2980 (8) Å
b = 10.0586 (9) Å
c = 19.2595 (17) Å
V = 1995.0 (3) Å^3
Z = 8
F(000) = 784
D_x = 1.220 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 10382 reflections
θ = 2.1–28.2°
μ = 0.09 mm^{-1}
T = 295 K
Block, colourless
0.18 × 0.16 × 0.14 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and *φ* scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.984, T_{max} = 0.987
9496 measured reflections
2394 independent reflections
1673 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 28.3°, θ_{min} = 2.1°
h = −13→12
k = −12→12
l = −24→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.143$
$S = 1.04$
2394 reflections
122 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
$w = 1/[\sigma^2(F_o^2) + (0.0681P)^2 + 0.4306P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.051 (4)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.07130 (13)	0.17170 (15)	0.67576 (7)	0.0411 (4)
C2	1.01976 (15)	0.06187 (15)	0.71025 (8)	0.0454 (4)
H2	0.9527	0.0140	0.6897	0.055*
C3	1.06624 (15)	0.02280 (16)	0.77417 (8)	0.0489 (4)
H3	1.0315	−0.0518	0.7959	0.059*
C4	1.16481 (14)	0.09434 (17)	0.80639 (8)	0.0463 (4)
C5	1.21388 (15)	0.20718 (16)	0.77404 (8)	0.0479 (4)
H5	1.2774	0.2579	0.7959	0.058*
C6	1.16815 (14)	0.24402 (15)	0.70933 (8)	0.0453 (4)
H6	1.2028	0.3187	0.6877	0.054*
C8	1.02545 (14)	0.21186 (16)	0.60471 (8)	0.0446 (4)
C9	1.3600 (3)	0.0899 (2)	0.54792 (15)	0.1060 (10)
H9A	1.4478	0.0611	0.5406	0.159*
H9B	1.3047	0.0507	0.5134	0.159*
H9C	1.3318	0.0627	0.5933	0.159*
C10	1.4471 (2)	0.3010 (3)	0.58929 (11)	0.0863 (7)
H10A	1.4299	0.2755	0.6364	0.129*
H10B	1.4385	0.3956	0.5848	0.129*
H10C	1.5338	0.2750	0.5770	0.129*
N1	1.35343 (14)	0.23451 (14)	0.54264 (7)	0.0525 (4)
H1A	1.2726	0.2616	0.5533	0.063*
H1B	1.3698	0.2589	0.4985	0.063*
O1	1.20733 (12)	0.05085 (14)	0.86889 (6)	0.0650 (4)
H1	1.2727	0.0922	0.8800	0.098*
O2	0.91717 (11)	0.16686 (14)	0.58397 (6)	0.0603 (4)
O3	1.09461 (11)	0.28636 (13)	0.56856 (6)	0.0590 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0336 (7)	0.0454 (8)	0.0441 (8)	0.0053 (6)	0.0039 (6)	−0.0005 (6)
C2	0.0371 (8)	0.0468 (9)	0.0524 (9)	−0.0036 (6)	−0.0020 (6)	−0.0028 (7)

C3	0.0422 (8)	0.0487 (9)	0.0557 (9)	−0.0063 (7)	0.0003 (7)	0.0073 (7)
C4	0.0363 (8)	0.0561 (9)	0.0465 (8)	0.0000 (7)	0.0001 (6)	0.0050 (7)
C5	0.0386 (8)	0.0518 (9)	0.0534 (9)	−0.0072 (7)	−0.0047 (6)	−0.0014 (7)
C6	0.0383 (8)	0.0442 (8)	0.0533 (9)	−0.0022 (6)	0.0027 (6)	0.0034 (6)
C8	0.0349 (8)	0.0524 (9)	0.0467 (8)	0.0063 (6)	0.0049 (6)	0.0011 (7)
C9	0.130 (2)	0.0600 (14)	0.128 (2)	0.0119 (14)	0.0553 (19)	0.0005 (14)
C10	0.0676 (13)	0.125 (2)	0.0665 (13)	−0.0039 (13)	−0.0052 (11)	−0.0110 (13)
N1	0.0505 (8)	0.0579 (9)	0.0492 (8)	0.0060 (6)	0.0098 (6)	0.0028 (6)
O1	0.0531 (7)	0.0878 (10)	0.0541 (7)	−0.0161 (6)	−0.0109 (5)	0.0198 (6)
O2	0.0446 (7)	0.0909 (10)	0.0454 (6)	−0.0114 (6)	−0.0022 (5)	0.0078 (6)
O3	0.0462 (7)	0.0713 (8)	0.0596 (7)	−0.0017 (6)	0.0014 (5)	0.0190 (6)

Geometric parameters (Å, º)

C1—C6	1.394 (2)	C8—O2	1.2680 (19)
C1—C2	1.394 (2)	C9—N1	1.460 (3)
C1—C8	1.503 (2)	C9—H9A	0.9600
C2—C3	1.378 (2)	C9—H9B	0.9600
C2—H2	0.9300	C9—H9C	0.9600
C3—C4	1.390 (2)	C10—N1	1.478 (3)
C3—H3	0.9300	C10—H10A	0.9600
C4—O1	1.3535 (19)	C10—H10B	0.9600
C4—C5	1.390 (2)	C10—H10C	0.9600
C5—C6	1.383 (2)	N1—H1A	0.9000
C5—H5	0.9300	N1—H1B	0.9000
C6—H6	0.9300	O1—H1	0.8200
C8—O3	1.2464 (19)		
C6—C1—C2	117.72 (14)	O2—C8—C1	117.85 (14)
C6—C1—C8	120.46 (14)	N1—C9—H9A	109.5
C2—C1—C8	121.82 (14)	N1—C9—H9B	109.5
C3—C2—C1	121.30 (14)	H9A—C9—H9B	109.5
C3—C2—H2	119.4	N1—C9—H9C	109.5
C1—C2—H2	119.4	H9A—C9—H9C	109.5
C2—C3—C4	120.30 (15)	H9B—C9—H9C	109.5
C2—C3—H3	119.8	N1—C10—H10A	109.5
C4—C3—H3	119.8	N1—C10—H10B	109.5
O1—C4—C5	123.02 (14)	H10A—C10—H10B	109.5
O1—C4—C3	117.76 (14)	N1—C10—H10C	109.5
C5—C4—C3	119.21 (14)	H10A—C10—H10C	109.5
C6—C5—C4	119.93 (14)	H10B—C10—H10C	109.5
C6—C5—H5	120.0	C9—N1—C10	112.2 (2)
C4—C5—H5	120.0	C9—N1—H1A	109.2
C5—C6—C1	121.47 (14)	C10—N1—H1A	109.2
C5—C6—H6	119.3	C9—N1—H1B	109.2
C1—C6—H6	119.3	C10—N1—H1B	109.2
O3—C8—O2	122.76 (15)	H1A—N1—H1B	107.9
O3—C8—C1	119.39 (14)	C4—O1—H1	109.5

C6—C1—C2—C3	−2.5 (2)	C4—C5—C6—C1	1.2 (2)
C8—C1—C2—C3	177.33 (14)	C2—C1—C6—C5	1.3 (2)
C1—C2—C3—C4	1.2 (2)	C8—C1—C6—C5	−178.54 (14)
C2—C3—C4—O1	−179.52 (15)	C6—C1—C8—O3	18.5 (2)
C2—C3—C4—C5	1.4 (2)	C2—C1—C8—O3	−161.34 (15)
O1—C4—C5—C6	178.38 (15)	C6—C1—C8—O2	−162.06 (15)
C3—C4—C5—C6	−2.5 (2)	C2—C1—C8—O2	18.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O3	0.90	1.87	2.7614 (18)	169
O1—H1···O2^{i}	0.82	1.81	2.6183 (17)	171
N1—H1*B*···O2^{ii}	0.90	1.82	2.7131 (17)	170

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