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2-Methylpropan-2-aminium 4-hydroxybenzoate

Shu-Lan Yu

Chemistry Engineering Department, Weifang Vocational College, Weifang 261000, People's Republic of China
Correspondence e-mail: crystal_wf@163.com

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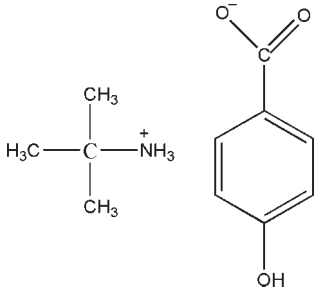
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.057; wR factor = 0.168; data-to-parameter ratio = 18.0.

In the crystal of the title molecular salt, $C_4H_{12}N^+\cdot C_7H_5O_3^-$, the cation is linked to three nearby anions by N—H···O hydrogen bonds. An O—H···O hydrogen bond between anions further consolidates the packing.

Related literature

For a related structure, see: Scholz & Gorls (2002).



Experimental

Crystal data

$C_4H_{12}N^+\cdot C_7H_5O_3^-$ M_r = 211.26
Monoclinic, $P2_1/c$
a = 6.8300 (14) Å
b = 9.2790 (19) Å
c = 19.831 (4) Å
β = 99.58 (3)°
V = 1239.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.10 × 0.09 × 0.08 mm

Data collection

Bruker SMART CCD diffractometer
2899 measured reflections
2677 independent reflections
1804 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.168
S = 1.04
2677 reflections
149 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···O1^{i}	0.82	1.83	2.621 (2)	163
N1—H1···O2^{ii}	0.92 (2)	1.93 (2)	2.835 (2)	168.2 (18)
N1—H3···O2	0.94 (2)	1.93 (2)	2.842 (2)	162.2 (18)
N1—H2···O1^{iii}	0.87 (2)	1.92 (3)	2.796 (2)	174.7 (19)

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5493).

References

Bruker (2003). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Scholz, J. & Gorls, H. (2002). *Polyhedron*, **21**, 305–312.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2010). E**66**, o1706 [doi:10.1107/S1600536810022592]

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S1. Experimental

A mixture of 2-methylpropan-2-amine(0.02 mol) and 4-hydroxybenzoic acid (0.02 mol) was stirred in ethanol (30 ml) at 353 K for 3 h to afford the title compound (yield 50%). Colourless bars of (I) were obtained by recrystallization from acetone at room temperature.

S2. Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H and C—H distances of 0.86 and 0.93–0.96 Å, respectively, and with U_{iso}(H) = 1.2U_{eq} of the parent atoms.

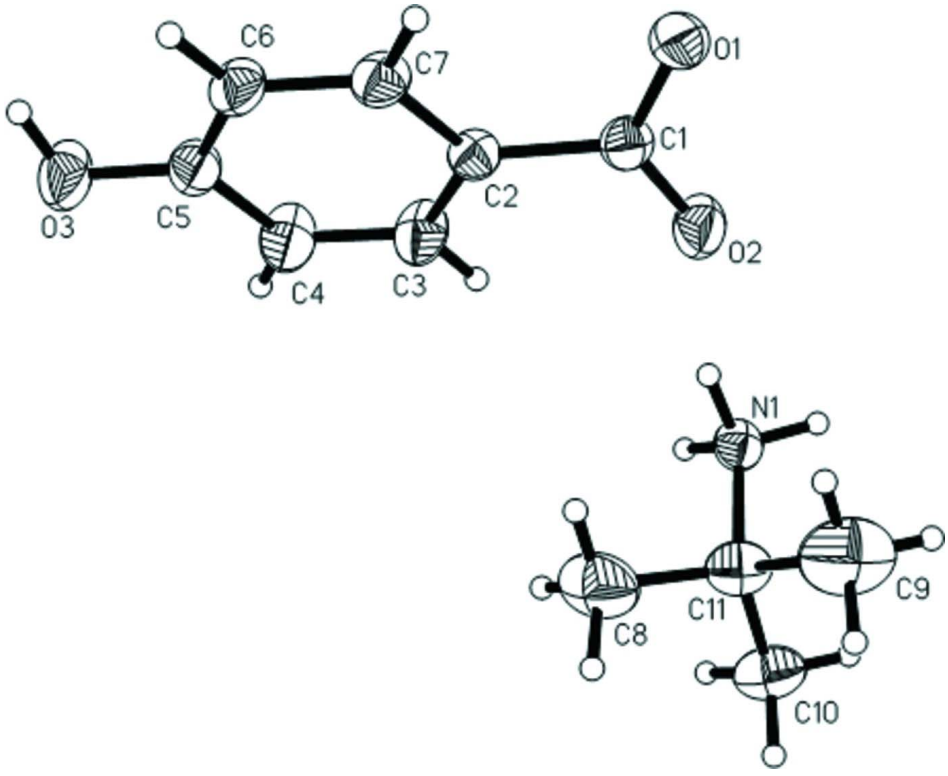

Figure 1

The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level.

2-Methylpropan-2-aminium 4-hydroxybenzoate

Crystal data

$C_4H_{12}N^+·C_7H_5O_3^-$
M_r = 211.26
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 6.8300 (14) Å
b = 9.2790 (19) Å
c = 19.831 (4) Å
β = 99.58 (3)°
V = 1239.3 (4) Å^3
Z = 4
$F(000)$ = 456
D_x = 1.132 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1804 reflections
θ = 2.1–27.0°
μ = 0.08 mm^{-1}
T = 293 K
Bar, colorless
0.10 × 0.09 × 0.08 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
2899 measured reflections
2677 independent reflections
1804 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.0°, θ_{min} = 2.1°
h = 0→8
k = 0→11
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.168
S = 1.04
2677 reflections
149 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0928P)^2 + 0.1735P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.59 (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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.1770 (3)	0.81042 (19)	0.40216 (9)	0.0475 (4)
C2	0.2054 (2)	0.70697 (18)	0.34696 (8)	0.0435 (4)
C3	0.3911 (3)	0.6882 (2)	0.32850 (10)	0.0618 (6)

H3A	0.4999	0.7372	0.3523	0.074*
C4	0.4170 (3)	0.5976 (3)	0.27512 (12)	0.0728 (7)
H4A	0.5423	0.5872	0.2632	0.087*
C5	0.2577 (3)	0.5225 (2)	0.23940 (10)	0.0571 (5)
C6	0.0722 (3)	0.5367 (2)	0.25849 (10)	0.0558 (5)
H6A	−0.0351	0.4843	0.2359	0.067*
C7	0.0470 (2)	0.6290 (2)	0.31113 (9)	0.0513 (5)
H7A	−0.0785	0.6393	0.3229	0.062*
O1	0.00062 (19)	0.84869 (15)	0.40644 (6)	0.0606 (4)
O2	0.3246 (2)	0.85859 (16)	0.44198 (7)	0.0667 (5)
O3	0.2922 (2)	0.4377 (2)	0.18682 (9)	0.0863 (6)
H3B	0.1865	0.4187	0.1622	0.129*
C8	0.7450 (4)	0.6075 (3)	0.50722 (16)	0.0949 (9)
H8A	0.6109	0.6040	0.4832	0.142*
H8B	0.7693	0.5259	0.5372	0.142*
H8C	0.8352	0.6053	0.4749	0.142*
C9	0.6313 (5)	0.7601 (4)	0.59955 (17)	0.1178 (12)
H9A	0.6486	0.8522	0.6218	0.177*
H9B	0.6563	0.6850	0.6331	0.177*
H9C	0.4977	0.7520	0.5754	0.177*
C10	0.9911 (4)	0.7600 (3)	0.58411 (13)	0.0806 (7)
H10A	1.0103	0.8519	0.6065	0.121*
H10B	1.0772	0.7522	0.5507	0.121*
H10C	1.0213	0.6845	0.6173	0.121*
C11	0.7764 (3)	0.7461 (2)	0.54907 (11)	0.0632 (6)
N1	0.7346 (2)	0.86993 (18)	0.49897 (8)	0.0483 (4)
H1	0.734 (3)	0.958 (2)	0.5202 (10)	0.058*
H2	0.815 (3)	0.869 (2)	0.4690 (12)	0.058*
H3	0.608 (3)	0.859 (2)	0.4718 (10)	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0461 (10)	0.0530 (10)	0.0442 (8)	0.0012 (8)	0.0095 (7)	0.0012 (7)
C2	0.0394 (9)	0.0475 (9)	0.0439 (8)	−0.0014 (7)	0.0077 (7)	0.0004 (7)
C3	0.0401 (10)	0.0804 (13)	0.0662 (11)	−0.0155 (9)	0.0120 (8)	−0.0224 (10)
C4	0.0406 (10)	0.1022 (17)	0.0781 (14)	−0.0061 (10)	0.0176 (9)	−0.0322 (12)
C5	0.0449 (10)	0.0678 (12)	0.0576 (10)	0.0055 (8)	0.0055 (8)	−0.0158 (9)
C6	0.0394 (9)	0.0673 (12)	0.0583 (10)	−0.0050 (8)	0.0008 (7)	−0.0132 (9)
C7	0.0356 (8)	0.0661 (11)	0.0523 (9)	−0.0023 (8)	0.0070 (7)	−0.0036 (8)
O1	0.0513 (8)	0.0813 (10)	0.0505 (7)	0.0161 (7)	0.0122 (6)	−0.0023 (6)
O2	0.0521 (8)	0.0788 (10)	0.0674 (9)	−0.0015 (7)	0.0051 (6)	−0.0267 (7)
O3	0.0537 (8)	0.1141 (13)	0.0890 (11)	0.0104 (8)	0.0058 (7)	−0.0525 (10)
C8	0.0918 (18)	0.0576 (14)	0.127 (2)	−0.0112 (12)	−0.0065 (16)	0.0126 (14)
C9	0.098 (2)	0.161 (3)	0.107 (2)	0.013 (2)	0.0542 (18)	0.056 (2)
C10	0.0671 (14)	0.0876 (16)	0.0802 (15)	0.0001 (12)	−0.0078 (12)	0.0154 (13)
C11	0.0545 (11)	0.0673 (12)	0.0678 (12)	−0.0024 (10)	0.0105 (9)	0.0151 (10)
N1	0.0421 (8)	0.0528 (9)	0.0510 (8)	−0.0009 (7)	0.0108 (7)	−0.0036 (7)

Geometric parameters (Å, º)

C1—O2	1.255 (2)	C8—H8A	0.9600
C1—O1	1.272 (2)	C8—H8B	0.9600
C1—C2	1.493 (2)	C8—H8C	0.9600
C2—C3	1.388 (2)	C9—C11	1.527 (3)
C2—C7	1.394 (2)	C9—H9A	0.9600
C3—C4	1.386 (3)	C9—H9B	0.9600
C3—H3A	0.9300	C9—H9C	0.9600
C4—C5	1.384 (3)	C10—C11	1.520 (3)
C4—H4A	0.9300	C10—H10A	0.9600
C5—O3	1.358 (2)	C10—H10B	0.9600
C5—C6	1.388 (3)	C10—H10C	0.9600
C6—C7	1.383 (3)	C11—N1	1.515 (2)
C6—H6A	0.9300	N1—H1	0.92 (2)
C7—H7A	0.9300	N1—H2	0.87 (2)
O3—H3B	0.8200	N1—H3	0.94 (2)
C8—C11	1.527 (3)		
O2—C1—O1	121.95 (16)	H8A—C8—H8C	109.5
O2—C1—C2	120.11 (16)	H8B—C8—H8C	109.5
O1—C1—C2	117.93 (15)	C11—C9—H9A	109.5
C3—C2—C7	117.80 (15)	C11—C9—H9B	109.5
C3—C2—C1	120.66 (15)	H9A—C9—H9B	109.5
C7—C2—C1	121.53 (15)	C11—C9—H9C	109.5
C4—C3—C2	121.05 (17)	H9A—C9—H9C	109.5
C4—C3—H3A	119.5	H9B—C9—H9C	109.5
C2—C3—H3A	119.5	C11—C10—H10A	109.5
C5—C4—C3	120.47 (18)	C11—C10—H10B	109.5
C5—C4—H4A	119.8	H10A—C10—H10B	109.5
C3—C4—H4A	119.8	C11—C10—H10C	109.5
O3—C5—C4	117.57 (17)	H10A—C10—H10C	109.5
O3—C5—C6	123.22 (17)	H10B—C10—H10C	109.5
C4—C5—C6	119.21 (17)	N1—C11—C10	107.33 (16)
C7—C6—C5	119.93 (16)	N1—C11—C8	106.78 (18)
C7—C6—H6A	120.0	C10—C11—C8	110.92 (19)
C5—C6—H6A	120.0	N1—C11—C9	107.08 (19)
C6—C7—C2	121.50 (16)	C10—C11—C9	112.0 (2)
C6—C7—H7A	119.3	C8—C11—C9	112.4 (2)
C2—C7—H7A	119.3	C11—N1—H1	113.0 (13)
C5—O3—H3B	109.5	C11—N1—H2	111.4 (13)
C11—C8—H8A	109.5	H1—N1—H2	111.9 (19)
C11—C8—H8B	109.5	C11—N1—H3	110.4 (12)
H8A—C8—H8B	109.5	H1—N1—H3	106.4 (18)
C11—C8—H8C	109.5	H2—N1—H3	103.3 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*B*···O1^{i}	0.82	1.83	2.621 (2)	163
N1—H1···O2^{ii}	0.92 (2)	1.93 (2)	2.835 (2)	168.2 (18)
N1—H3···O2	0.94 (2)	1.93 (2)	2.842 (2)	162.2 (18)
N1—H2···O1^{iii}	0.87 (2)	1.92 (3)	2.796 (2)	174.7 (19)

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