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1-Hydroxyisoquinolin-2-ium hydrogen succinate

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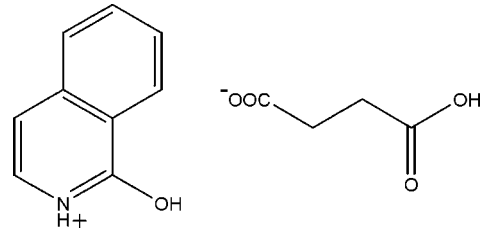
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.169; data-to-parameter ratio = 20.4.

In the title salt, $C_9H_8NO^+\cdot C_4H_5O_4^-$, the isoquinolinium ring system is approximately planar [r.m.s deviation = 0.011 (2) Å]. In the crystal, adjacent cations and anions are linked by O—H···O and N—H···O hydrogen bonds, forming columns along the b axis. The columns are connected by weak C—H···O interactions into a three-dimensional network.

Related literature

For the biological activity of quinoline derivatives, see: Hopkins *et al.* (2005); Musiol *et al.* (2006). For bond-length data, see: Allen *et al.* (1987). For a related quinoline structure, see: Loh *et al.* (2010).



Experimental

Crystal data

$C_9H_8NO^+\cdot C_4H_5O_4^-$
M_r = 263.24
Monoclinic, $P2_1$
a = 9.553 (5) Å
b = 4.962 (3) Å
c = 12.706 (5) Å
β = 104.117 (5)°
V = 584.1 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 295 K
0.22 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.975, T_{max} = 0.982
8297 measured reflections
3688 independent reflections
3289 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.169
S = 1.10
3688 reflections
181 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.92 (1)	2.48 (2)	3.255 (3)	142 (3)
O1—H1A···O4^{ii}	0.81 (1)	1.91 (1)	2.705 (2)	170 (3)
O2—H2A···O5^{iii}	0.83 (1)	1.77 (1)	2.591 (2)	169 (3)
C4—H4···O3^{iv}	0.93	2.50	3.360 (3)	154
C8—H8···O5^{v}	0.93	2.34	3.078 (3)	137
C9—H9···O4^{v}	0.93	1.81	2.718 (2)	165

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

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*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: IS5349).

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supporting information

Acta Cryst. (2014). E**70**, o491 [doi:10.1107/S1600536814006485]

1-Hydroxyisoquinolin-2-ium hydrogen succinate

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S1. Comment

Quinolinium derivatives are known to exhibit interesting bioactivities and pharmacological activities (Hopkins *et al.*, 2005; Musiol *et al.*, 2006). We herewith report the crystal structure of the title compound (Fig. 1). The bond lengths of the anion are within normal range (Allen *et al.*, 1987) and the bond lengths of cation are comparable with the reported similar structure (Loh *et al.*, 2010).

In the cation, the isoquinolinium ring system is planar [r.m.s deviation = 0.011 (2) Å]. The adjacent cations and anions are linked by weak intermolecular O—H···O and N—H···O interactions (Table 1 and Fig. 2) to form a column along the *b* axis. Weak π–π [*Cg*1···*Cg*1 (1-x, 1/2+y, -z) distance = 4.994 (3) Å, *Cg*1···*Cg*2 (x, -1+y, z) distance = 4.673 (3) Å; *Cg*1 and *Cg*2 are the centroids of the rings (N1/C1–C5) and (C1/C5–C9), respectively] and C—H···O interactions are also observed in the crystal structure.

S2. Experimental

1-Hydroxyisoquinolin-2-ium succinate was synthesized using the raw materials 1-hydroxyisoquinoline (1.45 g) and succinic acid (1.18 g) in an equimolar ratio. These reactants were dissolved in 10 ml of ethanol solvent and yellow precipitate was obtained after some time. The precipitate was dissolved in the same solvent and it is kept at room temperature for crystallization. After a span of four days, rod like crystals for diffraction study were harvested.

S3. Refinement

H atoms for $C_{aromatic}H$ and CH_2 were positioned geometrically and refined using riding model, with C—H = 0.93 and 0.97 Å, respectively, and with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms bounded to N and O atoms were located in a difference Fourier map and refined with $U_{iso}(H) = 1.5U_{eq}(N, O)$ and distance restraints of O—H = 0.82 (1) Å and N—H = 0.86 (1) Å. One reflection (0 0 1) was omited during refinement as it was showing poor agreement.

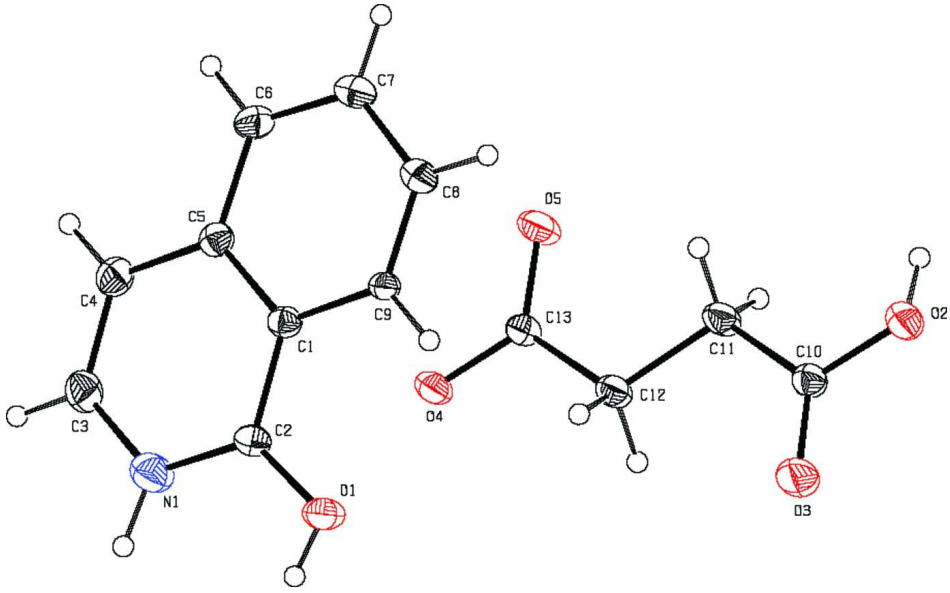

Figure 1

The molecular structure of the title cpompound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

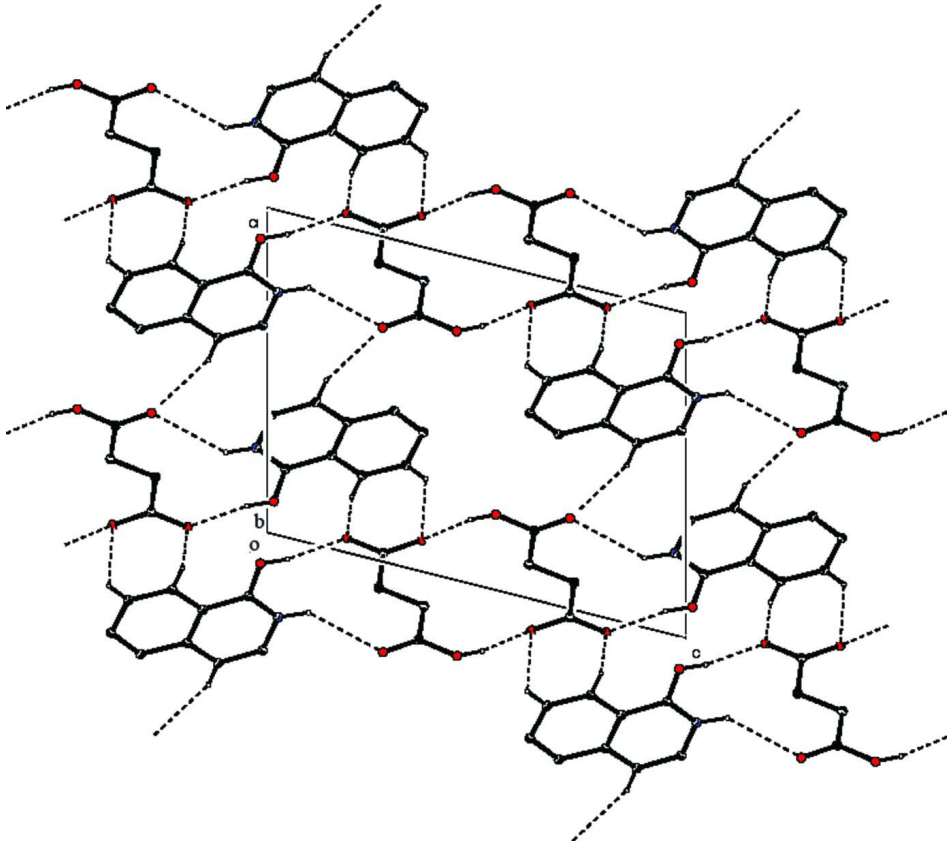

Figure 2

The packing diagram of the title compound, viewed down the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

1-Hydroxyisoquinolin-2-ium 3-carboxypropionate

Crystal data

$C_9H_8NO^+·C_4H_5O_4^-$
M_r = 263.24
Monoclinic, $P2_1$
Hall symbol: P 2yb
a = 9.553 (5) Å
b = 4.962 (3) Å
c = 12.706 (5) Å
β = 104.117 (5)°
V = 584.1 (5) Å^3
Z = 2
$F(000)$ = 276
D_x = 1.497 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4664 reflections
θ = 2.2–32.6°
μ = 0.12 mm^{-1}
T = 295 K
Block, colourless
0.22 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.975, T_{max} = 0.982
8297 measured reflections
3688 independent reflections
3289 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 33.2°, θ_{min} = 2.2°
h = −13→14
k = −6→7
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.169
S = 1.10
3688 reflections
181 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.1138P)^2 + 0.0584P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.28708 (17)	1.0029 (4)	0.15427 (13)	0.0248 (3)
C2	0.21024 (18)	1.0069 (4)	0.04383 (12)	0.0268 (3)
C3	0.3651 (2)	0.6470 (5)	0.01057 (17)	0.0378 (4)

H3	0.3901	0.5288	−0.0387	0.045*
C4	0.4391 (2)	0.6380 (4)	0.11717 (17)	0.0345 (4)
H4	0.5135	0.5146	0.1404	0.041*
C5	0.40134 (18)	0.8183 (4)	0.19153 (14)	0.0273 (3)
C6	0.4726 (2)	0.8221 (5)	0.30338 (15)	0.0352 (4)
H6	0.5492	0.7052	0.3300	0.042*
C7	0.4292 (2)	0.9972 (5)	0.37231 (14)	0.0381 (4)
H7	0.4749	0.9978	0.4459	0.046*
C8	0.3161 (2)	1.1745 (5)	0.33147 (14)	0.0342 (4)
H8	0.2870	1.2942	0.3783	0.041*
C9	0.24902 (16)	1.1760 (3)	0.22686 (11)	0.0219 (3)
H9	0.1742	1.2977	0.2021	0.026*
C10	−0.2126 (2)	1.2254 (4)	0.36224 (13)	0.0294 (4)
C11	−0.1045 (2)	0.9998 (5)	0.37431 (13)	0.0337 (4)
H11A	−0.1356	0.8529	0.4136	0.040*
H11B	−0.0122	1.0633	0.4174	0.040*
C12	−0.0841 (2)	0.8927 (4)	0.26675 (13)	0.0303 (3)
H12A	−0.1760	0.8251	0.2246	0.036*
H12B	−0.0559	1.0410	0.2266	0.036*
C13	0.02711 (18)	0.6711 (4)	0.27745 (12)	0.0258 (3)
N1	0.2522 (2)	0.8310 (5)	−0.02600 (14)	0.0423 (4)
H1	0.214 (3)	0.848 (9)	−0.0992 (9)	0.063*
O1	0.10057 (16)	1.1826 (3)	0.01569 (11)	0.0364 (3)
H1A	0.067 (3)	1.149 (7)	−0.0474 (11)	0.055*
O2	−0.23278 (17)	1.3291 (4)	0.45355 (11)	0.0410 (4)
H2A	−0.198 (3)	1.257 (7)	0.5134 (15)	0.061*
O3	−0.27879 (19)	1.3135 (5)	0.27647 (12)	0.0492 (5)
O4	0.04477 (15)	0.5692 (3)	0.19024 (9)	0.0332 (3)
O5	0.09610 (18)	0.5944 (4)	0.36893 (10)	0.0425 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0245 (7)	0.0250 (7)	0.0242 (6)	−0.0023 (6)	0.0042 (5)	0.0003 (6)
C2	0.0285 (8)	0.0263 (8)	0.0234 (6)	−0.0023 (7)	0.0023 (5)	−0.0009 (6)
C3	0.0405 (10)	0.0367 (10)	0.0375 (9)	0.0019 (8)	0.0118 (7)	−0.0097 (8)
C4	0.0335 (8)	0.0329 (10)	0.0371 (9)	0.0060 (7)	0.0088 (7)	0.0011 (7)
C5	0.0259 (7)	0.0275 (8)	0.0284 (6)	−0.0007 (7)	0.0064 (6)	0.0019 (6)
C6	0.0308 (8)	0.0414 (11)	0.0305 (7)	0.0065 (8)	0.0015 (6)	0.0067 (7)
C7	0.0390 (10)	0.0474 (12)	0.0246 (7)	0.0031 (9)	0.0010 (6)	0.0000 (8)
C8	0.0363 (9)	0.0406 (10)	0.0244 (7)	0.0025 (8)	0.0048 (6)	−0.0041 (7)
C9	0.0215 (6)	0.0236 (7)	0.0190 (5)	0.0008 (6)	0.0022 (5)	−0.0010 (5)
C10	0.0318 (8)	0.0310 (9)	0.0251 (6)	0.0048 (7)	0.0065 (6)	0.0020 (6)
C11	0.0425 (10)	0.0346 (9)	0.0219 (6)	0.0133 (8)	0.0038 (6)	0.0019 (6)
C12	0.0359 (9)	0.0322 (9)	0.0215 (6)	0.0067 (7)	0.0047 (6)	0.0013 (6)
C13	0.0290 (7)	0.0249 (8)	0.0220 (6)	0.0003 (6)	0.0036 (5)	−0.0006 (5)
N1	0.0468 (10)	0.0450 (11)	0.0331 (7)	−0.0002 (9)	0.0058 (7)	−0.0062 (8)
O1	0.0384 (7)	0.0378 (8)	0.0273 (6)	0.0087 (6)	−0.0031 (5)	−0.0047 (5)

O2	0.0439 (8)	0.0501 (9)	0.0283 (6)	0.0138 (7)	0.0077 (5)	−0.0033 (6)
O3	0.0540 (9)	0.0608 (12)	0.0310 (6)	0.0270 (9)	0.0069 (6)	0.0116 (7)
O4	0.0389 (7)	0.0384 (8)	0.0205 (5)	0.0064 (6)	0.0036 (4)	−0.0035 (5)
O5	0.0549 (9)	0.0469 (9)	0.0213 (5)	0.0213 (8)	0.0010 (5)	−0.0017 (5)

Geometric parameters (Å, º)

C1—C9	1.373 (2)	C8—H8	0.9300
C1—C5	1.415 (2)	C9—H9	0.9300
C1—C2	1.416 (2)	C10—O3	1.201 (2)
C2—O1	1.343 (2)	C10—O2	1.325 (2)
C2—N1	1.372 (2)	C10—C11	1.506 (3)
C3—C4	1.367 (3)	C11—C12	1.522 (2)
C3—N1	1.403 (3)	C11—H11A	0.9700
C3—H3	0.9300	C11—H11B	0.9700
C4—C5	1.410 (3)	C12—C13	1.512 (3)
C4—H4	0.9300	C12—H12A	0.9700
C5—C6	1.418 (2)	C12—H12B	0.9700
C6—C7	1.368 (3)	C13—O5	1.248 (2)
C6—H6	0.9300	C13—O4	1.266 (2)
C7—C8	1.392 (3)	N1—H1	0.917 (10)
C7—H7	0.9300	O1—H1A	0.806 (10)
C8—C9	1.327 (2)	O2—H2A	0.833 (10)
C9—C1—C5	119.31 (14)	C8—C9—H9	119.1
C9—C1—C2	119.92 (15)	C1—C9—H9	119.1
C5—C1—C2	120.77 (15)	O3—C10—O2	119.75 (18)
O1—C2—N1	124.95 (15)	O3—C10—C11	124.01 (17)
O1—C2—C1	117.06 (15)	O2—C10—C11	116.24 (15)
N1—C2—C1	117.98 (16)	C10—C11—C12	113.75 (14)
C4—C3—N1	121.27 (18)	C10—C11—H11A	108.8
C4—C3—H3	119.4	C12—C11—H11A	108.8
N1—C3—H3	119.4	C10—C11—H11B	108.8
C3—C4—C5	119.22 (18)	C12—C11—H11B	108.8
C3—C4—H4	120.4	H11A—C11—H11B	107.7
C5—C4—H4	120.4	C13—C12—C11	114.45 (14)
C4—C5—C1	119.27 (16)	C13—C12—H12A	108.6
C4—C5—C6	122.75 (18)	C11—C12—H12A	108.6
C1—C5—C6	117.98 (16)	C13—C12—H12B	108.6
C7—C6—C5	120.24 (18)	C11—C12—H12B	108.6
C7—C6—H6	119.9	H12A—C12—H12B	107.6
C5—C6—H6	119.9	O5—C13—O4	122.73 (17)
C6—C7—C8	119.46 (16)	O5—C13—C12	120.36 (14)
C6—C7—H7	120.3	O4—C13—C12	116.91 (14)
C8—C7—H7	120.3	C2—N1—C3	121.47 (16)
C9—C8—C7	121.22 (18)	C2—N1—H1	119 (3)
C9—C8—H8	119.4	C3—N1—H1	119 (2)
C7—C8—H8	119.4	C2—O1—H1A	103 (2)

C8—C9—C1	121.79 (17)	C10—O2—H2A	122 (2)
C9—C1—C2—O1	−0.7 (2)	C5—C6—C7—C8	−1.0 (3)
C5—C1—C2—O1	178.07 (16)	C6—C7—C8—C9	0.3 (3)
C9—C1—C2—N1	179.79 (17)	C7—C8—C9—C1	0.3 (3)
C5—C1—C2—N1	−1.5 (3)	C5—C1—C9—C8	−0.3 (3)
N1—C3—C4—C5	−0.2 (3)	C2—C1—C9—C8	178.46 (18)
C3—C4—C5—C1	0.4 (3)	O3—C10—C11—C12	0.7 (3)
C3—C4—C5—C6	179.99 (19)	O2—C10—C11—C12	−178.94 (18)
C9—C1—C5—C4	179.17 (17)	C10—C11—C12—C13	178.42 (17)
C2—C1—C5—C4	0.4 (3)	C11—C12—C13—O5	−1.7 (3)
C9—C1—C5—C6	−0.4 (2)	C11—C12—C13—O4	177.79 (17)
C2—C1—C5—C6	−179.14 (17)	O1—C2—N1—C3	−177.81 (19)
C4—C5—C6—C7	−178.5 (2)	C1—C2—N1—C3	1.7 (3)
C1—C5—C6—C7	1.1 (3)	C4—C3—N1—C2	−0.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.92 (1)	2.48 (2)	3.255 (3)	142 (3)
O1—H1*A*···O4^{ii}	0.81 (1)	1.91 (1)	2.705 (2)	170 (3)
O2—H2*A*···O5^{iii}	0.83 (1)	1.77 (1)	2.591 (2)	169 (3)
C4—H4···O3^{iv}	0.93	2.50	3.360 (3)	154
C8—H8···O5^{v}	0.93	2.34	3.078 (3)	137
C9—H9···O4^{v}	0.93	1.81	2.718 (2)	165

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