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2-Aminopyridinium 2-hydroxy-2,2-diphenylacetate

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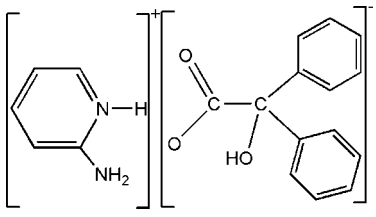
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.125; data-to-parameter ratio = 14.0.

In the title salt, $C_5H_7N_2^+\cdot C_{14}H_{11}O_3^-$, the cation and anion interact through N—H···O hydrogen bonds involving the protonated NH group of the cation and the hydroxyl group of the anion. Both H atoms of the NH_2 group in the cation are engaged in N—H···O hydrogen bonds with the carbonyl groups of two symmetry-related anions, forming an infinite one-dimensional chain in the [100] direction.

Related literature

For related literature, see: Banerjee *et al.* (2006); Zeng *et al.* (2005).



Experimental

Crystal data

$C_5H_7N_2^+\cdot C_{14}H_{11}O_3^-$
M_r = 322.35
Monoclinic, $P2_1/c$
a = 10.041 (2) Å
b = 14.371 (3) Å
c = 11.953 (3) Å
β = 104.714 (3)°
V = 1668.1 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.42 × 0.16 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.964, T_{max} = 0.991
8927 measured reflections
3261 independent reflections
2373 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.125
S = 1.06
3261 reflections
233 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 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—H1A···O3	0.868 (9)	1.870 (10)	2.7264 (19)	168.6 (19)
N2—H2A···O1^{i}	0.860 (9)	2.020 (10)	2.879 (2)	179.2 (18)
N2—H2B···O2^{ii}	0.869 (9)	1.965 (11)	2.820 (2)	167.4 (19)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2138).

References

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  doi:10.1107/S1600536807050787

supplementary materials

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2-Aminopyridinium 2-hydroxy-2,2-diphenylacetate

J. Li, H. Li and L. Sui

Comment

Rational design and synthesis of supramolecular architectures using hydrogen bonding interactions is still a hot field due to intriguing topologies and potential applications in opto-electronics and catalysis (Banerjee *et al.*, 2006). A number of reports have been published in past decades (Zeng *et al.*, 2005). Herein we present the structure of a supramolecular salt, 2-aminopyridinium 2-hydroxy-2,2-diphenylacetate, (I).

The asymmetric unit of the title salt consists of one 2-aminopyridinium cation and one 2-hydroxy-2,2-diphenylacetate anion, in which ions are connected through a N—H···O hydrogen bond (Table 1, entry 1). Within the anion, a weak contact between H3A and O1 is observed, generating a *S*(5) ring (Fig. 1 and Table 1). Finally, both amine H atoms in the cation link symmetry related anions through *N*—*H*···*O*(carbonyl) hydrogen bonds, giving an infinite one-dimensional chain along the direction [100], as shown in Fig. 2.

Experimental

All reagents were commercially available and of analytical grade. A 5 ml e thanol solution of 2-aminopyridine (1.0 mmol, 0.094 g) was added to a 20 ml hot aqueous solution of 2-hydroxy-2,2-diphenylacetic acid (1.0 mmol, 0.23 g), and the mixture was stirred for 10 min. at 373 K. Then the solution was filtered, and the filtrate was kept at room temperature. After one week, colourless crystals of (I) were obtained.

Refinement

H atoms bonded to N and O atoms were located in a difference map and refined isotropically with restrained bond lengths: N—H = 0.85 (1) Å and O—H = 0.82 (1). Other H atoms were placed in calculated positions and were refined as riding atoms with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(carrier C).

Figures

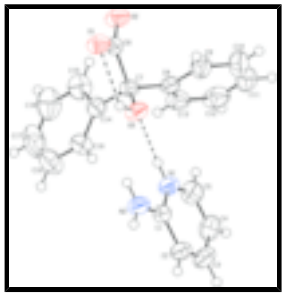

Fig. 1. The asymmetric unit of (I). Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

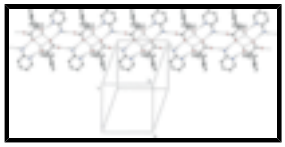

Fig. 2. An infinite one-dimensional chain along the [100] axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity.

2-Aminopyridinium 2-hydroxy-2,2-diphenylacetate

Crystal data

$C_5H_7N_2^+ \cdot C_{14}H_{11}O_3^-$	$F_{000} = 680$
$M_r = 322.35$	$D_x = 1.284$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 5480 reflections
$a = 10.041$ (2) Å	$\theta = 2.5$–28.3º
$b = 14.371$ (3) Å	$\mu = 0.09$ mm^{-1}
$c = 11.953$ (3) Å	$T = 298$ (2) K
$\beta = 104.714$ (3)º	Needle, colourless
$V = 1668.1$ (7) Å^3	0.42 × 0.16 × 0.10 mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3261 independent reflections
Radiation source: fine-focus sealed tube	2373 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.027$
$T = 298$(2) K	$\theta_{max} = 26.0$º
ω scans	$\theta_{min} = 2.1$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -12 \rightarrow 12$
$T_{min} = 0.964$, $T_{max} = 0.991$	$k = -17 \rightarrow 14$
8927 measured reflections	$l = -10 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.125$	$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.2552P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
3261 reflections	$\Delta\rho_{max} = 0.15$ e Å^{-3}
233 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
4 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}
N1	0.66548 (15)	0.18811 (10)	0.79894 (13)	0.0464 (4)
H1A	0.6111 (17)	0.1582 (13)	0.8324 (15)	0.066 (6)*
N2	0.85192 (18)	0.10260 (11)	0.90008 (14)	0.0510 (4)
H2A	0.7976 (16)	0.0720 (11)	0.9318 (14)	0.051 (5)*
H2B	0.9385 (11)	0.0888 (14)	0.9113 (17)	0.064 (6)*
O1	0.32779 (13)	0.00093 (8)	0.99259 (10)	0.0499 (3)
O2	0.12570 (12)	0.05947 (9)	0.89953 (11)	0.0554 (4)
O3	0.46608 (12)	0.10383 (8)	0.88096 (10)	0.0462 (3)
H3A	0.492 (2)	0.0586 (10)	0.9239 (15)	0.068 (7)*
C1	0.80094 (18)	0.16810 (11)	0.82341 (14)	0.0392 (4)
C2	0.88145 (19)	0.21943 (12)	0.76463 (15)	0.0480 (5)
H2	0.9756	0.2084	0.7793	0.058*
C3	0.8215 (2)	0.28468 (13)	0.68688 (17)	0.0579 (5)
H3	0.8753	0.3185	0.6485	0.069*
C4	0.6804 (2)	0.30249 (14)	0.66276 (17)	0.0601 (5)
H4	0.6396	0.3470	0.6083	0.072*
C5	0.6054 (2)	0.25355 (14)	0.72046 (18)	0.0575 (5)
H5	0.5114	0.2646	0.7065	0.069*
C6	0.25153 (17)	0.04849 (11)	0.91492 (14)	0.0372 (4)
C7	0.32230 (16)	0.09481 (11)	0.82693 (13)	0.0373 (4)
C8	0.27078 (17)	0.19414 (12)	0.79965 (14)	0.0396 (4)
C9	0.2831 (2)	0.25527 (12)	0.89119 (17)	0.0564 (5)
H9	0.3197	0.2342	0.9663	0.068*
C10	0.2424 (3)	0.34656 (14)	0.8732 (2)	0.0756 (7)
H10	0.2500	0.3862	0.9359	0.091*
C11	0.1907 (3)	0.37923 (15)	0.7633 (2)	0.0764 (7)
H11	0.1640	0.4412	0.7513	0.092*
C12	0.1784 (2)	0.32063 (16)	0.6711 (2)	0.0680 (6)
H12	0.1439	0.3428	0.5962	0.082*
C13	0.21746 (19)	0.22771 (13)	0.68924 (16)	0.0524 (5)
H13	0.2075	0.1879	0.6263	0.063*
C14	0.3004 (2)	0.03108 (12)	0.72152 (15)	0.0461 (4)
C15	0.1700 (2)	0.00022 (15)	0.66520 (17)	0.0635 (6)
H15	0.0941	0.0203	0.6898	0.076*
C16	0.1519 (3)	−0.06039 (17)	0.5723 (2)	0.0840 (8)
H16	0.0640	−0.0810	0.5352	0.101*
C17	0.2633 (4)	−0.09008 (17)	0.5349 (2)	0.0937 (9)
H17	0.2508	−0.1307	0.4725	0.112*
C18	0.3916 (4)	−0.06006 (18)	0.5889 (2)	0.0891 (8)
H18	0.4670	−0.0799	0.5633	0.107*
C19	0.4104 (2)	−0.00005 (14)	0.68190 (18)	0.0640 (6)
H19	0.4989	0.0198	0.7186	0.077*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0403 (9)	0.0447 (9)	0.0575 (9)	−0.0038 (7)	0.0186 (7)	0.0045 (7)
N2	0.0472 (10)	0.0529 (10)	0.0582 (10)	0.0026 (8)	0.0231 (8)	0.0141 (8)
O1	0.0464 (7)	0.0562 (8)	0.0500 (7)	0.0097 (6)	0.0174 (6)	0.0208 (6)
O2	0.0392 (7)	0.0659 (9)	0.0660 (9)	0.0063 (6)	0.0220 (6)	0.0166 (7)
O3	0.0346 (7)	0.0519 (8)	0.0523 (7)	0.0023 (6)	0.0114 (6)	0.0184 (6)
C1	0.0411 (10)	0.0374 (9)	0.0413 (9)	−0.0027 (7)	0.0147 (7)	−0.0022 (7)
C2	0.0435 (10)	0.0498 (11)	0.0547 (11)	−0.0058 (8)	0.0195 (9)	0.0039 (9)
C3	0.0660 (14)	0.0535 (12)	0.0581 (12)	−0.0147 (10)	0.0231 (10)	0.0083 (9)
C4	0.0677 (14)	0.0478 (11)	0.0602 (12)	0.0020 (10)	0.0079 (10)	0.0127 (9)
C5	0.0464 (11)	0.0539 (12)	0.0691 (13)	0.0055 (9)	0.0090 (10)	0.0061 (10)
C6	0.0391 (10)	0.0347 (9)	0.0401 (9)	0.0024 (7)	0.0142 (7)	0.0020 (7)
C7	0.0339 (9)	0.0420 (9)	0.0370 (9)	0.0039 (7)	0.0110 (7)	0.0070 (7)
C8	0.0367 (9)	0.0406 (9)	0.0447 (9)	0.0010 (7)	0.0160 (7)	0.0099 (7)
C9	0.0735 (14)	0.0438 (11)	0.0524 (11)	−0.0004 (10)	0.0169 (10)	0.0030 (9)
C10	0.1036 (19)	0.0426 (12)	0.0858 (17)	0.0020 (12)	0.0335 (14)	0.0005 (11)
C11	0.0910 (18)	0.0438 (12)	0.1058 (19)	0.0132 (11)	0.0459 (15)	0.0213 (13)
C12	0.0679 (14)	0.0692 (14)	0.0724 (14)	0.0177 (11)	0.0277 (11)	0.0388 (12)
C13	0.0541 (11)	0.0582 (12)	0.0489 (10)	0.0105 (9)	0.0202 (9)	0.0150 (9)
C14	0.0574 (12)	0.0404 (9)	0.0428 (10)	0.0053 (8)	0.0169 (9)	0.0069 (8)
C15	0.0679 (14)	0.0661 (13)	0.0516 (12)	0.0014 (11)	0.0064 (10)	−0.0016 (10)
C16	0.107 (2)	0.0689 (15)	0.0620 (14)	−0.0041 (14)	−0.0038 (14)	−0.0077 (12)
C17	0.163 (3)	0.0606 (15)	0.0581 (15)	0.0115 (18)	0.0289 (18)	−0.0135 (12)
C18	0.130 (3)	0.0702 (16)	0.0835 (18)	0.0126 (16)	0.0579 (18)	−0.0136 (14)
C19	0.0782 (15)	0.0563 (12)	0.0699 (13)	0.0022 (11)	0.0413 (12)	−0.0052 (10)

Geometric parameters (Å, °)

N1—C1	1.348 (2)	C8—C9	1.384 (2)
N1—C5	1.357 (2)	C9—C10	1.375 (3)
N1—H1A	0.868 (9)	C9—H9	0.9300
N2—C1	1.323 (2)	C10—C11	1.366 (3)
N2—H2A	0.860 (9)	C10—H10	0.9300
N2—H2B	0.869 (9)	C11—C12	1.367 (3)
O1—C6	1.2467 (18)	C11—H11	0.9300
O2—C6	1.240 (2)	C12—C13	1.393 (3)
O3—C7	1.430 (2)	C12—H12	0.9300
O3—H3A	0.829 (9)	C13—H13	0.9300
C1—C2	1.407 (2)	C14—C19	1.382 (3)
C2—C3	1.350 (3)	C14—C15	1.384 (3)
C2—H2	0.9300	C15—C16	1.386 (3)
C3—C4	1.395 (3)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.374 (4)
C4—C5	1.342 (3)	C16—H16	0.9300
C4—H4	0.9300	C17—C18	1.357 (4)
C5—H5	0.9300	C17—H17	0.9300

C6—C7	1.560 (2)	C18—C19	1.381 (3)
C7—C8	1.525 (2)	C18—H18	0.9300
C7—C14	1.528 (2)	C19—H19	0.9300
C8—C13	1.379 (2)		
C1—N1—C5	123.01 (16)	C10—C9—C8	121.23 (19)
C1—N1—H1A	120.9 (14)	C10—C9—H9	119.4
C5—N1—H1A	116.1 (14)	C8—C9—H9	119.4
C1—N2—H2A	119.5 (12)	C11—C10—C9	120.2 (2)
C1—N2—H2B	117.8 (14)	C11—C10—H10	119.9
H2A—N2—H2B	122.5 (19)	C9—C10—H10	119.9
C7—O3—H3A	109.6 (15)	C10—C11—C12	119.8 (2)
N2—C1—N1	119.59 (16)	C10—C11—H11	120.1
N2—C1—C2	123.28 (17)	C12—C11—H11	120.1
N1—C1—C2	117.12 (16)	C11—C12—C13	120.0 (2)
C3—C2—C1	119.71 (17)	C11—C12—H12	120.0
C3—C2—H2	120.1	C13—C12—H12	120.0
C1—C2—H2	120.1	C8—C13—C12	120.6 (2)
C2—C3—C4	121.45 (18)	C8—C13—H13	119.7
C2—C3—H3	119.3	C12—C13—H13	119.7
C4—C3—H3	119.3	C19—C14—C15	117.98 (19)
C5—C4—C3	118.05 (18)	C19—C14—C7	121.10 (17)
C5—C4—H4	121.0	C15—C14—C7	120.89 (17)
C3—C4—H4	121.0	C14—C15—C16	120.4 (2)
C4—C5—N1	120.64 (19)	C14—C15—H15	119.8
C4—C5—H5	119.7	C16—C15—H15	119.8
N1—C5—H5	119.7	C17—C16—C15	120.2 (3)
O2—C6—O1	126.18 (16)	C17—C16—H16	119.9
O2—C6—C7	117.85 (14)	C15—C16—H16	119.9
O1—C6—C7	115.92 (14)	C18—C17—C16	120.0 (2)
O3—C7—C8	105.10 (13)	C18—C17—H17	120.0
O3—C7—C14	110.13 (13)	C16—C17—H17	120.0
C8—C7—C14	114.51 (13)	C17—C18—C19	120.0 (3)
O3—C7—C6	108.35 (12)	C17—C18—H18	120.0
C8—C7—C6	110.83 (13)	C19—C18—H18	120.0
C14—C7—C6	107.78 (13)	C18—C19—C14	121.4 (2)
C13—C8—C9	118.00 (17)	C18—C19—H19	119.3
C13—C8—C7	124.07 (16)	C14—C19—H19	119.3
C9—C8—C7	117.89 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O3	0.868 (9)	1.870 (10)	2.7264 (19)	168.6 (19)
N2—H2A···O1^{i}	0.860 (9)	2.020 (10)	2.879 (2)	179.2 (18)
N2—H2B···O2^{ii}	0.869 (9)	1.965 (11)	2.820 (2)	167.4 (19)
O3—H3A···O1	0.829 (9)	2.19 (2)	2.6147 (17)	112.2 (17)
O3—H3A···O1^{i}	0.829 (9)	2.018 (16)	2.6917 (17)	138.0 (19)

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

Fig. 1

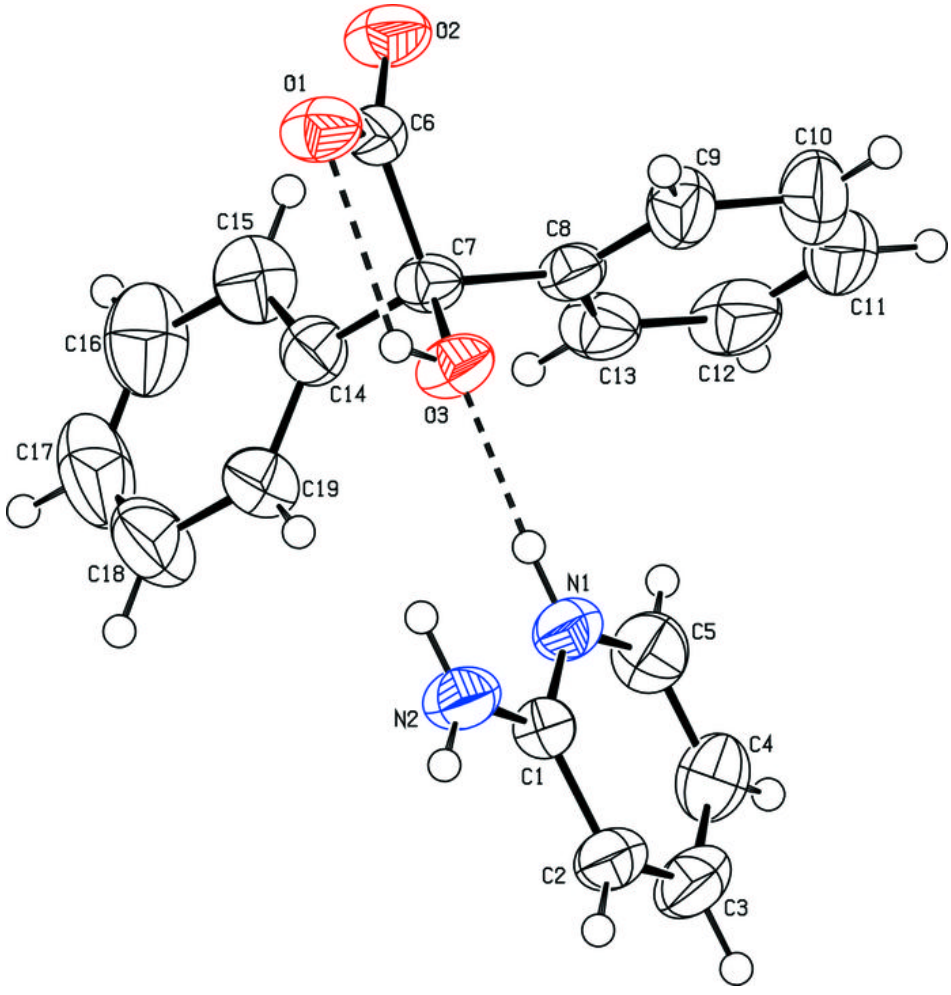
O2
O1
C6
C9
C10
C15
C8
C7
C11
C16
C13
C12
C14
O3
C17
C19
C18
N1
C5
N2
C4
C1
C2
C3

Fig. 2