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2-Methylpyridinium benzylate

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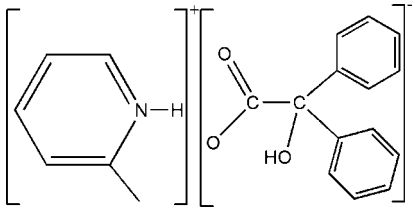
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.057; wR factor = 0.156; data-to-parameter ratio = 14.4.

The asymmetric unit of the title salt, $C_6H_8N^+\cdot C_{14}H_{11}O_3^-$, contains two pairs of 2-methylpyridinium cations and benzylate anions, in which the cation links to the anion through an N—H···O hydrogen bond. An intramolecular O—H···O bond occurs in each benzylate anion and constructs an S(6) ring. The anions are linked into centrosymmetric dimers by further O—H···O hydrogen bonds.

Related literature

For related literature, see: Zhang & Chen (2005).



Experimental

Crystal data

$C_6H_8N^+\cdot C_{14}H_{11}O_3^-$
M_r = 321.36
Triclinic, $P\overline{1}$
a = 8.411 (6) Å
b = 12.342 (8) Å
c = 16.291 (11) Å
α = 91.93 (1)°
β = 90.10 (1)°
γ = 95.77 (1)°
V = 1682 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.45 × 0.21 × 0.12 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.963, T_{max} = 0.990
9222 measured reflections
6472 independent reflections
4128 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.156
S = 0.99
6472 reflections
451 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 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···O4	0.864 (8)	1.757 (8)	2.6155 (19)	172.0 (13)
N2—H2A···O1	0.862 (8)	1.748 (8)	2.6081 (19)	176.6 (14)
O3—H3···O2	0.816 (8)	2.123 (13)	2.5870 (19)	116.0 (11)
O3—H3···O2^{i}	0.816 (8)	2.158 (9)	2.909 (2)	153.1 (13)
O6—H6···O5	0.829 (8)	2.053 (15)	2.5748 (19)	120.4 (14)
O6—H6···O5^{ii}	0.829 (8)	2.167 (11)	2.904 (2)	148.0 (16)

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

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: HB2553).

References

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supplementary materials

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2-Methylpyridinium benzylate

J. Li

Comment

Supramolecular hydrogen-bonded molecular networks are of great current interest (Zhang & Chen, 2005). In this paper, we report the title supramolecular salt, (I), in which the component ions are connected by hydrogen bonds.

Compound (I) contains two pairs of 2-methylpyridinium anions and benzylate anions, in which each 2-methylpyridinium anion interacts with its adjacent benzylate anion through an intermolecular N—H···O hydrogen bond (Fig. 1 and Table 1). In addition, an intramolecular O—H···O hydrogen bond also exists in each benzylate anion and forms an S(6) ring. These O—H···O bonds are bifurcated to nearby O atoms, thus forming inversion dimers.

Experimental

10 ml 2-methylpyridine was added to a 20-ml hot aqueous solution of benzylic acid (1.0 mmol, 0.23 g) and the mixture was stirred for 10 minutes under the temperature of 373 K. Then, the solution was filtered, and the filtrate was kept at room temperature. After 5 d, colorless crystals of (I) were obtained.

Refinement

The N– and O-bound H atoms were located in a difference map and refined with distance restraints N—H = 0.86 (1)Å and O—H = 0.82 (1) Å; their U_{iso} values were freely refined.

The C-bound H atoms were placed in calculated positions (C—H = 0.93–0.96 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

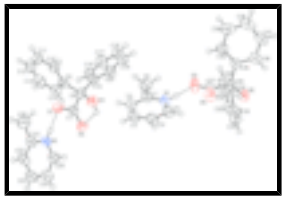


Fig. 1. The molecular structure of (I). Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

2-Methylpyridinium benzylate

Crystal data

$C_6H_8N^+·C_{14}H_{11}O_3^-$	$Z = 4$
$M_r = 321.36$	$F_{000} = 680$

Triclinic, $P\bar{1}$	D_x = 1.269 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.411 (6) Å	Cell parameters from 3910 reflections
b = 12.342 (8) Å	θ = 2.5–28.2º
c = 16.291 (11) Å	μ = 0.09 mm^{-1}
α = 91.93 (1)º	T = 298 (2) K
β = 90.10 (1)º	Block, colourless
γ = 95.77 (1)º	0.45 × 0.21 × 0.12 mm
V = 1682 (2) Å^3	

Data collection

Bruker SMART APEX CCD diffractometer	6472 independent reflections
Radiation source: fine-focus sealed tube	4128 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
T = 298(2) K	θ_{max} = 26.0º
ω scans	θ_{min} = 1.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	h = −10→9
T_{min} = 0.963, T_{max} = 0.990	k = −15→14
9222 measured reflections	l = −20→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)]$ = 0.057	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.156	$w = 1/[\sigma^2(F_o^2) + (0.0823P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max}$ = 0.005
6472 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
451 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *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}
N1	0.55457 (15)	0.82749 (9)	0.75636 (7)	0.0485 (3)
H1A	0.5007 (14)	0.8084 (11)	0.7996 (6)	0.078 (5)*
N2	0.89574 (15)	0.81387 (10)	0.26014 (7)	0.0502 (3)
H2A	0.9425 (15)	0.7909 (11)	0.3023 (6)	0.091 (6)*
O1	1.04816 (13)	0.74676 (8)	0.38526 (6)	0.0570 (3)
O2	0.98770 (13)	0.90310 (8)	0.43913 (6)	0.0596 (3)
O3	1.21228 (13)	0.91798 (7)	0.54884 (6)	0.0521 (3)
H3	1.1438 (11)	0.9577 (9)	0.5379 (9)	0.082 (6)*
O4	0.38038 (14)	0.75371 (8)	0.87914 (6)	0.0632 (3)
O5	0.47755 (13)	0.91188 (8)	0.93295 (6)	0.0621 (3)
O6	0.25502 (13)	0.92267 (7)	1.04037 (6)	0.0494 (3)
H6	0.3435 (10)	0.9560 (12)	1.0315 (11)	0.113 (7)*
C1	0.57741 (19)	0.75707 (11)	0.69531 (8)	0.0497 (4)
C2	0.6699 (2)	0.79273 (13)	0.63023 (9)	0.0661 (5)
H2	0.6880	0.7448	0.5868	0.079*
C3	0.7350 (2)	0.89825 (14)	0.62927 (10)	0.0703 (5)
H3A	0.7974	0.9224	0.5851	0.084*
C4	0.7087 (2)	0.96873 (14)	0.69324 (10)	0.0691 (5)
H4	0.7526	1.0410	0.6932	0.083*
C5	0.6171 (2)	0.93118 (13)	0.75678 (9)	0.0599 (5)
H5	0.5979	0.9780	0.8008	0.072*
C6	0.5010 (2)	0.64462 (12)	0.70150 (10)	0.0716 (6)
H6A	0.4730	0.6313	0.7576	0.107*
H6B	0.5740	0.5941	0.6829	0.107*
H6C	0.4063	0.6353	0.6680	0.107*
C7	1.05986 (17)	0.82215 (11)	0.43985 (8)	0.0400 (4)
C8	1.17637 (17)	0.81246 (10)	0.51333 (8)	0.0403 (4)
C9	1.33132 (17)	0.77351 (10)	0.48098 (8)	0.0407 (4)
C10	1.35768 (19)	0.66546 (11)	0.47539 (9)	0.0500 (4)
H10	1.2806	0.6130	0.4943	0.060*
C11	1.4980 (2)	0.63371 (13)	0.44183 (9)	0.0606 (5)
H11	1.5139	0.5602	0.4385	0.073*
C12	1.6127 (2)	0.70919 (14)	0.41370 (9)	0.0655 (5)
H12	1.7066	0.6878	0.3911	0.079*
C13	1.5875 (2)	0.81688 (14)	0.41924 (10)	0.0651 (5)
H13	1.6651	0.8692	0.4005	0.078*
C14	1.4494 (2)	0.84836 (12)	0.45196 (9)	0.0535 (4)
H14	1.4344	0.9220	0.4548	0.064*
C15	1.09641 (17)	0.73823 (10)	0.57771 (8)	0.0416 (4)
C16	0.9994 (2)	0.64452 (12)	0.55794 (9)	0.0556 (5)
H16	0.9780	0.6247	0.5031	0.067*
C17	0.9334 (2)	0.57936 (13)	0.61955 (10)	0.0674 (5)

H17	0.8690	0.5157	0.6057	0.081*
C18	0.9622 (2)	0.60797 (13)	0.70014 (10)	0.0677 (5)
H18	0.9160	0.5645	0.7410	0.081*
C19	1.0583 (2)	0.69983 (14)	0.72092 (10)	0.0681 (5)
H19	1.0784	0.7191	0.7759	0.082*
C20	1.1260 (2)	0.76461 (12)	0.66033 (9)	0.0553 (5)
H20	1.1926	0.8270	0.6750	0.066*
C21	0.85741 (19)	0.74396 (12)	0.19715 (9)	0.0508 (4)
C22	0.7842 (2)	0.78106 (13)	0.12961 (9)	0.0632 (5)
H22	0.7579	0.7339	0.0849	0.076*
C23	0.7499 (2)	0.88649 (14)	0.12772 (10)	0.0720 (6)
H23	0.6987	0.9110	0.0822	0.086*
C24	0.7913 (2)	0.95657 (14)	0.19350 (10)	0.0689 (5)
H24	0.7699	1.0290	0.1930	0.083*
C25	0.8642 (2)	0.91750 (12)	0.25919 (9)	0.0584 (5)
H25	0.8925	0.9638	0.3042	0.070*
C26	0.8965 (2)	0.63068 (13)	0.20524 (11)	0.0757 (6)
H26A	0.9899	0.6196	0.1735	0.114*
H26B	0.8083	0.5811	0.1855	0.114*
H26C	0.9166	0.6177	0.2619	0.114*
C27	0.38621 (17)	0.82880 (11)	0.93368 (8)	0.0417 (4)
C28	0.26647 (17)	0.81715 (10)	1.00538 (8)	0.0396 (4)
C29	0.10108 (17)	0.77338 (10)	0.97282 (8)	0.0385 (4)
C30	0.05481 (19)	0.66345 (11)	0.96260 (9)	0.0498 (4)
H30	0.1252	0.6136	0.9768	0.060*
C31	−0.0947 (2)	0.62605 (12)	0.93151 (9)	0.0577 (5)
H31	−0.1241	0.5515	0.9256	0.069*
C32	−0.1989 (2)	0.69766 (13)	0.90959 (9)	0.0600 (5)
H32	−0.2998	0.6724	0.8893	0.072*
C33	−0.1539 (2)	0.80724 (13)	0.91777 (9)	0.0590 (5)
H33	−0.2238	0.8567	0.9022	0.071*
C34	−0.00477 (19)	0.84452 (12)	0.94907 (8)	0.0496 (4)
H34	0.0246	0.9191	0.9542	0.060*
C35	0.32473 (17)	0.74434 (11)	1.07113 (8)	0.0432 (4)
C36	0.2938 (2)	0.76866 (13)	1.15287 (9)	0.0605 (5)
H36	0.2389	0.8285	1.1662	0.073*
C37	0.3424 (3)	0.70632 (14)	1.21463 (10)	0.0775 (6)
H37	0.3202	0.7241	1.2691	0.093*
C38	0.4231 (3)	0.61854 (14)	1.19611 (11)	0.0818 (6)
H38	0.4566	0.5765	1.2379	0.098*
C39	0.4550 (2)	0.59202 (13)	1.11579 (11)	0.0749 (6)
H39	0.5091	0.5315	1.1031	0.090*
C40	0.4066 (2)	0.65565 (12)	1.05309 (10)	0.0580 (5)
H40	0.4298	0.6380	0.9988	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

N1	0.0511 (8)	0.0545 (7)	0.0395 (6)	0.0025 (6)	0.0054 (6)	0.0026 (5)
N2	0.0504 (8)	0.0606 (7)	0.0397 (6)	0.0054 (6)	−0.0038 (6)	0.0044 (6)
O1	0.0706 (7)	0.0528 (6)	0.0489 (6)	0.0175 (5)	−0.0211 (5)	−0.0124 (5)
O2	0.0695 (7)	0.0553 (6)	0.0569 (6)	0.0238 (5)	−0.0166 (5)	−0.0080 (5)
O3	0.0620 (7)	0.0362 (5)	0.0573 (6)	0.0051 (5)	−0.0152 (5)	−0.0084 (4)
O4	0.0648 (7)	0.0619 (6)	0.0568 (6)	−0.0168 (5)	0.0180 (5)	−0.0168 (5)
O5	0.0608 (7)	0.0591 (6)	0.0601 (6)	−0.0213 (5)	0.0128 (5)	−0.0099 (5)
O6	0.0534 (6)	0.0391 (5)	0.0539 (6)	−0.0013 (5)	0.0063 (5)	−0.0090 (4)
C1	0.0552 (9)	0.0529 (8)	0.0428 (8)	0.0141 (7)	−0.0048 (7)	0.0021 (7)
C2	0.0813 (12)	0.0758 (11)	0.0440 (9)	0.0200 (9)	0.0126 (8)	0.0052 (8)
C3	0.0750 (12)	0.0837 (11)	0.0527 (9)	0.0042 (10)	0.0154 (9)	0.0216 (8)
C4	0.0778 (13)	0.0662 (10)	0.0604 (10)	−0.0102 (9)	0.0049 (9)	0.0125 (8)
C5	0.0700 (11)	0.0560 (9)	0.0512 (9)	−0.0049 (8)	0.0038 (8)	−0.0006 (7)
C6	0.0946 (14)	0.0561 (10)	0.0630 (10)	0.0032 (10)	0.0064 (10)	−0.0004 (8)
C7	0.0410 (8)	0.0408 (7)	0.0381 (7)	0.0031 (6)	−0.0007 (6)	0.0011 (6)
C8	0.0467 (8)	0.0334 (7)	0.0394 (7)	0.0002 (6)	−0.0065 (6)	−0.0062 (6)
C9	0.0412 (8)	0.0430 (7)	0.0365 (7)	−0.0009 (6)	−0.0084 (6)	−0.0011 (6)
C10	0.0515 (9)	0.0446 (8)	0.0523 (9)	0.0001 (7)	0.0020 (7)	−0.0045 (7)
C11	0.0624 (11)	0.0581 (9)	0.0625 (10)	0.0151 (8)	0.0036 (8)	−0.0076 (8)
C12	0.0497 (10)	0.0891 (12)	0.0570 (10)	0.0067 (9)	0.0065 (8)	−0.0052 (9)
C13	0.0515 (10)	0.0780 (11)	0.0626 (10)	−0.0102 (9)	0.0055 (8)	0.0072 (9)
C14	0.0540 (10)	0.0502 (8)	0.0547 (9)	−0.0032 (8)	−0.0033 (8)	0.0048 (7)
C15	0.0412 (8)	0.0429 (7)	0.0412 (7)	0.0080 (6)	−0.0041 (6)	−0.0027 (6)
C16	0.0639 (11)	0.0548 (9)	0.0451 (8)	−0.0065 (8)	0.0040 (8)	−0.0065 (7)
C17	0.0726 (12)	0.0584 (10)	0.0685 (11)	−0.0081 (9)	0.0087 (9)	0.0047 (8)
C18	0.0841 (13)	0.0673 (10)	0.0526 (9)	0.0080 (10)	0.0131 (9)	0.0153 (8)
C19	0.0848 (13)	0.0802 (11)	0.0397 (8)	0.0088 (10)	0.0012 (8)	0.0052 (8)
C20	0.0634 (11)	0.0584 (9)	0.0430 (8)	0.0027 (8)	−0.0064 (7)	−0.0034 (7)
C21	0.0503 (9)	0.0575 (9)	0.0439 (8)	0.0011 (7)	−0.0013 (7)	0.0039 (7)
C22	0.0740 (12)	0.0750 (11)	0.0390 (8)	−0.0006 (9)	−0.0113 (8)	0.0046 (8)
C23	0.0811 (13)	0.0871 (12)	0.0499 (9)	0.0129 (10)	−0.0096 (9)	0.0196 (9)
C24	0.0871 (13)	0.0672 (10)	0.0552 (10)	0.0165 (10)	−0.0029 (9)	0.0143 (8)
C25	0.0689 (11)	0.0569 (9)	0.0499 (9)	0.0084 (8)	−0.0045 (8)	0.0014 (7)
C26	0.0916 (14)	0.0651 (11)	0.0710 (11)	0.0138 (10)	−0.0158 (10)	−0.0054 (9)
C27	0.0405 (8)	0.0405 (7)	0.0427 (8)	−0.0025 (6)	−0.0033 (6)	0.0003 (6)
C28	0.0414 (8)	0.0367 (7)	0.0399 (7)	0.0007 (6)	0.0002 (6)	−0.0030 (6)
C29	0.0399 (8)	0.0402 (7)	0.0348 (7)	0.0006 (6)	0.0018 (6)	0.0025 (6)
C30	0.0474 (9)	0.0452 (8)	0.0565 (9)	0.0009 (7)	−0.0078 (7)	0.0082 (7)
C31	0.0567 (10)	0.0550 (9)	0.0575 (9)	−0.0141 (8)	−0.0099 (8)	0.0053 (7)
C32	0.0454 (10)	0.0782 (11)	0.0539 (9)	−0.0056 (9)	−0.0076 (8)	0.0013 (8)
C33	0.0500 (10)	0.0737 (10)	0.0552 (9)	0.0166 (8)	−0.0096 (8)	0.0002 (8)
C34	0.0545 (10)	0.0473 (8)	0.0478 (8)	0.0083 (7)	−0.0014 (7)	0.0015 (7)
C35	0.0414 (8)	0.0443 (8)	0.0419 (8)	−0.0060 (7)	−0.0055 (6)	0.0013 (6)
C36	0.0647 (11)	0.0680 (10)	0.0482 (9)	0.0017 (9)	−0.0006 (8)	0.0062 (8)
C37	0.1015 (16)	0.0827 (12)	0.0470 (9)	−0.0014 (11)	−0.0054 (10)	0.0135 (9)
C38	0.0991 (15)	0.0725 (11)	0.0719 (11)	−0.0086 (11)	−0.0303 (11)	0.0287 (9)
C39	0.0767 (13)	0.0532 (10)	0.0953 (13)	0.0076 (9)	−0.0244 (11)	0.0110 (9)
C40	0.0602 (10)	0.0539 (9)	0.0598 (9)	0.0059 (8)	−0.0107 (8)	0.0012 (8)

Geometric parameters (Å, °)

N1—C1	1.3259 (18)	C17—C18	1.363 (2)
N1—C5	1.334 (2)	C17—H17	0.9300
N1—H1A	0.864 (8)	C18—C19	1.357 (2)
N2—C25	1.333 (2)	C18—H18	0.9300
N2—C21	1.3361 (19)	C19—C20	1.379 (2)
N2—H2A	0.862 (8)	C19—H19	0.9300
O1—C7	1.2617 (16)	C20—H20	0.9300
O2—C7	1.2204 (17)	C21—C22	1.374 (2)
O3—C8	1.4113 (17)	C21—C26	1.478 (2)
O3—H3	0.816 (8)	C22—C23	1.362 (2)
O4—C27	1.2594 (17)	C22—H22	0.9300
O5—C27	1.2183 (17)	C23—C24	1.376 (2)
O6—C28	1.4163 (17)	C23—H23	0.9300
O6—H6	0.829 (8)	C24—C25	1.359 (2)
C1—C2	1.374 (2)	C24—H24	0.9300
C1—C6	1.476 (2)	C25—H25	0.9300
C2—C3	1.362 (2)	C26—H26A	0.9600
C2—H2	0.9300	C26—H26B	0.9600
C3—C4	1.368 (2)	C26—H26C	0.9600
C3—H3A	0.9300	C27—C28	1.545 (2)
C4—C5	1.358 (2)	C28—C29	1.528 (2)
C4—H4	0.9300	C28—C35	1.532 (2)
C5—H5	0.9300	C29—C30	1.378 (2)
C6—H6A	0.9600	C29—C34	1.376 (2)
C6—H6B	0.9600	C30—C31	1.384 (2)
C6—H6C	0.9600	C30—H30	0.9300
C7—C8	1.561 (2)	C31—C32	1.362 (2)
C8—C9	1.523 (2)	C31—H31	0.9300
C8—C15	1.5279 (19)	C32—C33	1.369 (2)
C9—C14	1.382 (2)	C32—H32	0.9300
C9—C10	1.374 (2)	C33—C34	1.382 (2)
C10—C11	1.388 (2)	C33—H33	0.9300
C10—H10	0.9300	C34—H34	0.9300
C11—C12	1.363 (2)	C35—C40	1.374 (2)
C11—H11	0.9300	C35—C36	1.386 (2)
C12—C13	1.367 (2)	C36—C37	1.373 (2)
C12—H12	0.9300	C36—H36	0.9300
C13—C14	1.365 (2)	C37—C38	1.361 (3)
C13—H13	0.9300	C37—H37	0.9300
C14—H14	0.9300	C38—C39	1.372 (3)
C15—C16	1.375 (2)	C38—H38	0.9300
C15—C20	1.390 (2)	C39—C40	1.394 (2)
C16—C17	1.389 (2)	C39—H39	0.9300
C16—H16	0.9300	C40—H40	0.9300
C1—N1—C5	122.62 (13)	C20—C19—H19	120.1
C1—N1—H1A	121.9 (9)	C15—C20—C19	121.15 (15)

C5—N1—H1A	115.4 (9)	C15—C20—H20	119.4
C25—N2—C21	121.89 (13)	C19—C20—H20	119.4
C25—N2—H2A	119.5 (9)	N2—C21—C22	118.51 (15)
C21—N2—H2A	118.6 (9)	N2—C21—C26	117.26 (14)
C8—O3—H3	111.4 (9)	C22—C21—C26	124.23 (14)
C28—O6—H6	104.1 (11)	C23—C22—C21	120.48 (15)
N1—C1—C2	118.39 (14)	C23—C22—H22	119.8
N1—C1—C6	117.65 (14)	C21—C22—H22	119.8
C2—C1—C6	123.96 (14)	C22—C23—C24	119.61 (16)
C3—C2—C1	120.08 (15)	C22—C23—H23	120.2
C3—C2—H2	120.0	C24—C23—H23	120.2
C1—C2—H2	120.0	C25—C24—C23	118.48 (16)
C2—C3—C4	119.95 (16)	C25—C24—H24	120.8
C2—C3—H3A	120.0	C23—C24—H24	120.8
C4—C3—H3A	120.0	N2—C25—C24	121.03 (15)
C5—C4—C3	118.69 (16)	N2—C25—H25	119.5
C5—C4—H4	120.7	C24—C25—H25	119.5
C3—C4—H4	120.7	C21—C26—H26A	109.5
N1—C5—C4	120.28 (15)	C21—C26—H26B	109.5
N1—C5—H5	119.9	H26A—C26—H26B	109.5
C4—C5—H5	119.9	C21—C26—H26C	109.5
C1—C6—H6A	109.5	H26A—C26—H26C	109.5
C1—C6—H6B	109.5	H26B—C26—H26C	109.5
H6A—C6—H6B	109.5	O5—C27—O4	124.52 (14)
C1—C6—H6C	109.5	O5—C27—C28	117.26 (12)
H6A—C6—H6C	109.5	O4—C27—C28	118.20 (12)
H6B—C6—H6C	109.5	O6—C28—C29	107.76 (11)
O2—C7—O1	124.76 (13)	O6—C28—C27	107.54 (10)
O2—C7—C8	117.27 (11)	C29—C28—C27	109.94 (11)
O1—C7—C8	117.96 (12)	O6—C28—C35	109.09 (11)
O3—C8—C9	107.94 (11)	C29—C28—C35	111.47 (11)
O3—C8—C15	109.00 (11)	C27—C28—C35	110.91 (12)
C9—C8—C15	112.85 (11)	C30—C29—C34	117.69 (14)
O3—C8—C7	107.33 (10)	C30—C29—C28	122.26 (13)
C9—C8—C7	109.21 (11)	C34—C29—C28	119.99 (13)
C15—C8—C7	110.34 (12)	C29—C30—C31	121.06 (14)
C14—C9—C10	117.42 (14)	C29—C30—H30	119.5
C14—C9—C8	119.53 (13)	C31—C30—H30	119.5
C10—C9—C8	122.98 (12)	C32—C31—C30	120.43 (15)
C11—C10—C9	120.79 (14)	C32—C31—H31	119.8
C11—C10—H10	119.6	C30—C31—H31	119.8
C9—C10—H10	119.6	C33—C32—C31	119.34 (16)
C12—C11—C10	120.67 (16)	C33—C32—H32	120.3
C12—C11—H11	119.7	C31—C32—H32	120.3
C10—C11—H11	119.7	C32—C33—C34	120.18 (15)
C11—C12—C13	118.87 (17)	C32—C33—H33	119.9
C11—C12—H12	120.6	C34—C33—H33	119.9
C13—C12—H12	120.6	C33—C34—C29	121.27 (15)
C12—C13—C14	120.61 (16)	C33—C34—H34	119.4

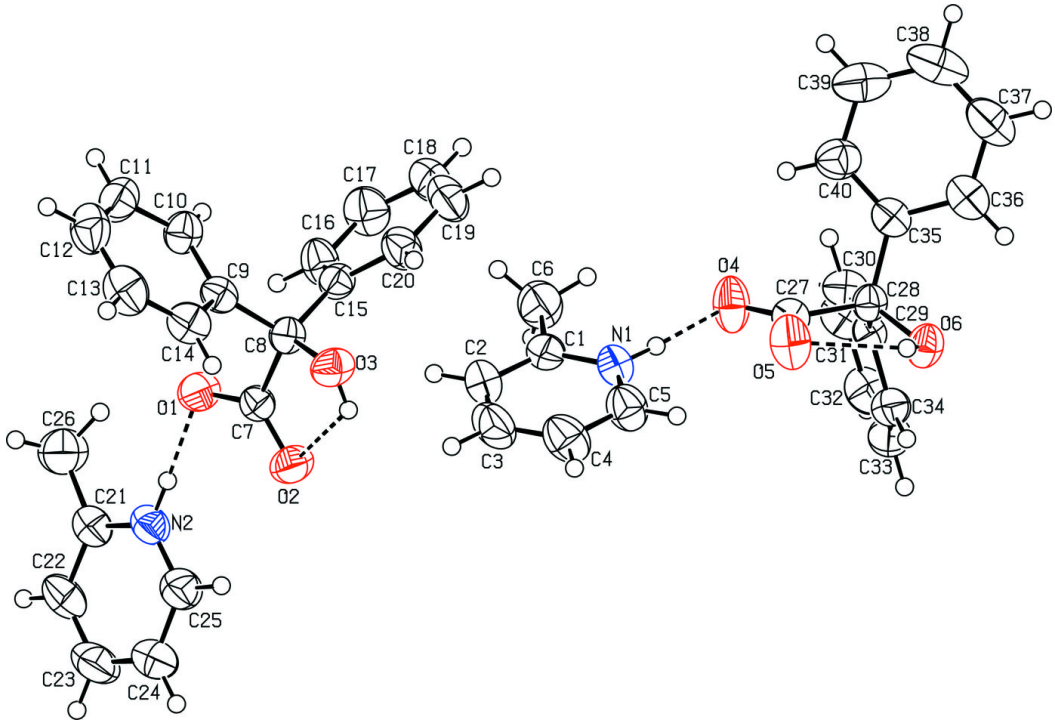
C12—C13—H13	119.7	C29—C34—H34	119.4
C14—C13—H13	119.7	C40—C35—C36	118.14 (14)
C13—C14—C9	121.65 (15)	C40—C35—C28	123.16 (13)
C13—C14—H14	119.2	C36—C35—C28	118.70 (13)
C9—C14—H14	119.2	C37—C36—C35	121.48 (16)
C16—C15—C20	118.07 (13)	C37—C36—H36	119.3
C16—C15—C8	123.16 (12)	C35—C36—H36	119.3
C20—C15—C8	118.76 (13)	C38—C37—C36	119.93 (17)
C15—C16—C17	120.20 (14)	C38—C37—H37	120.0
C15—C16—H16	119.9	C36—C37—H37	120.0
C17—C16—H16	119.9	C37—C38—C39	120.03 (17)
C18—C17—C16	120.57 (16)	C37—C38—H38	120.0
C18—C17—H17	119.7	C39—C38—H38	120.0
C16—C17—H17	119.7	C38—C39—C40	120.08 (17)
C17—C18—C19	120.13 (15)	C38—C39—H39	120.0
C17—C18—H18	119.9	C40—C39—H39	120.0
C19—C18—H18	119.9	C35—C40—C39	120.34 (16)
C18—C19—C20	119.87 (15)	C35—C40—H40	119.8
C18—C19—H19	120.1	C39—C40—H40	119.8

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O4	0.864 (8)	1.757 (8)	2.6155 (19)	172.0 (13)
N2—H2A···O1	0.862 (8)	1.748 (8)	2.6081 (19)	176.6 (14)
O3—H3···O2	0.816 (8)	2.123 (13)	2.5870 (19)	116.0 (11)
O3—H3···O2^{i}	0.816 (8)	2.158 (9)	2.909 (2)	153.1 (13)
O6—H6···O5	0.829 (8)	2.053 (15)	2.5748 (19)	120.4 (14)
O6—H6···O5^{ii}	0.829 (8)	2.167 (11)	2.904 (2)	148.0 (16)

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

Fig. 1


C38
C39
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O4
C27
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C7
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C26
C21
N2
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C25
C23
C24
C6
C1
N1
C2
C5
C3
C4