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4-(4-Aminobenzyl)anilinium 2-hydroxy-2,2-diphenylacetate

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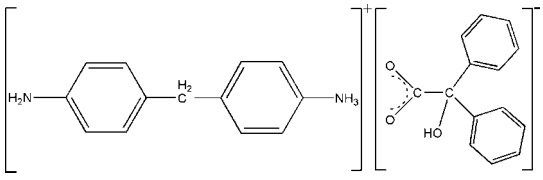
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.058; wR factor = 0.151; data-to-parameter ratio = 7.6.

The title compound, $C_{13}H_{15}N_2^+\cdot C_{14}H_{11}O_3^-$, is a molecular salt in which the conformation of the anion is stabilized by an intramolecular O—H···O interaction. The species are linked by an N—H···O bond and further hydrogen bonds lead to infinite one-dimensional chains along [010].

Related literature

For related literature, see: Li (2007); Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{13}H_{15}N_2^+\cdot C_{14}H_{11}O_3^-$
M_r = 426.50
Monoclinic, $P2_1$
a = 13.336 (6) Å
b = 6.477 (3) Å
c = 14.454 (7) Å
β = 114.777 (7)°
V = 1133.6 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.35 × 0.12 × 0.09 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.972, T_{max} = 0.993
5069 measured reflections
2385 independent reflections
1701 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.151
S = 1.06
2385 reflections
313 parameters
67 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.827 (9)	1.984 (19)	2.586 (3)	129 (2)
N2—H2C···O2^{i}	0.905 (10)	1.851 (11)	2.756 (3)	177.5 (18)
N2—H2B···O1^{ii}	0.903 (9)	1.818 (11)	2.711 (3)	170 (3)
N2—H2A···O1	0.904 (9)	1.865 (9)	2.759 (3)	169.6 (19)

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

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: HB2574).

References

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supplementary materials

Acta Cryst. (2007). E**63**, o4303 [**doi:10.1107/S1600536807049331**]

4-(4-Aminobenzyl)anilinium 2-hydroxy-2,2-diphenylacetate

J. Li

Comment

This work continues our previous synthetic and structural studies of hydrogen bonding interactions between the 2-hydroxy-2,2-diphenylacetate anion and substituted pyridinium cations (Li, 2007).

The asymmetric unit of the title compound, (I), contains one 4,4'-methylene bis(benzenammonium) cation and one 2-hydroxy-2,2-diphenylacetate anion, in which these component ions are linked together through an N—H···O hydrogen bond (Table 1, Fig. 1). The dihedral angles between the aromatic ring planes in the cation and the anion are 83.87 (18)° and 75.48 (17)°, respectively. An intramolecular O–H···O hydrogen bond occurs within the benzylate anion and a S(5) ring (Bernstein *et al.*, 1995) is generated. Moreover, adjacent ion pairs are further extended into an infinite one-dimensional chain along [010] by further intermolecular N—H···O hydrogen bonds (Fig. 2).

Experimental

A 5-ml ethanol solution of 4,4'-methylene bis(benzenamine) (1.0 mmol, 0.20 g) added to a 20-ml hot aqueous solution of benzylic acid (1.0 mmol, 0.23 g) and the mixture was stirred for 15 minutes under the temperature of 373 K. Then the solution was filtered, and the filtrate was kept at the room temperature. After a week, colorless blades of (I) were obtained.

Refinement

Anomalous dispersion was negligible and Friedel pairs were merged before refinement. H atoms bonded to nitrogen atoms and hydroxyl group were located in a difference synthesis and refined isotropically with N—H = 0.90 (1) Å and O—H = 0.82 (1) Å, respectively. All the remaining H atoms were placed in calculated positions, with C—H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively, and were refined as riding with $U_{iso} = 1.2U_{eq}$(C).

Figures

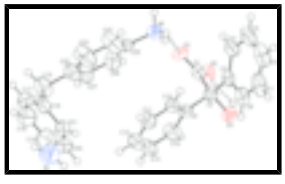

Fig. 1. The molecular structure of (I). Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

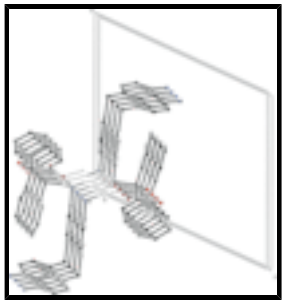

Fig. 2. An infinite one dimensional hydrogen bonded chain along [010]. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity.

4-(4-Aminobenzyl)anilinium 2-hydroxy-2,2-diphenylacetate

Crystal data

$C_{13}H_{15}N_2^+ \cdot C_{14}H_{11}O_3^-$	$F_{000} = 452$
$M_r = 426.50$	$D_x = 1.250$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 2500 reflections
$a = 13.336$ (6) Å	$\theta = 2.3$–28.2º
$b = 6.477$ (3) Å	$\mu = 0.08$ mm^{-1}
$c = 14.454$ (7) Å	$T = 298$ (2) K
$\beta = 114.777$ (7)º	Blade, colourless
$V = 1133.6$ (9) Å^3	0.35 × 0.12 × 0.09 mm
$Z = 2$	

Data collection

Bruker SMART APEX CCD diffractometer	2385 independent reflections
Radiation source: fine-focus sealed tube	1701 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.034$
$T = 298$(2) K	$\theta_{max} = 26.0$º
ω scans	$\theta_{min} = 1.7$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -16 \rightarrow 14$
$T_{min} = 0.972$, $T_{max} = 0.993$	$k = -7 \rightarrow 6$
5069 measured reflections	$l = -12 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.059$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.151$	$w = 1/[\sigma^2(F_o^2) + (0.0779P)^2 + 0.0728P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.06	$(\Delta/\sigma)_{max}$ = 0.005
2385 reflections	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
313 parameters	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
67 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 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}
N1	0.7443 (3)	−0.0297 (6)	0.4427 (2)	0.0852 (4)
H1A	0.7667 (13)	−0.121 (3)	0.4114 (13)	0.0836 (5)*
H1B	0.7345 (14)	0.038 (3)	0.4904 (11)	0.0836 (5)*
N2	0.08804 (18)	0.6545 (3)	0.07426 (16)	0.0424 (7)
H2A	0.0770 (14)	0.7807 (16)	0.0951 (14)	0.031 (7)*
H2B	0.0346 (14)	0.636 (5)	0.0108 (9)	0.067 (10)*
H2C	0.0708 (13)	0.558 (2)	0.1107 (13)	0.073 (11)*
O1	0.05811 (15)	1.0586 (3)	0.11769 (13)	0.0446 (5)
O2	0.03234 (17)	1.3555 (3)	0.18013 (16)	0.0609 (6)
O3	0.09565 (15)	1.2283 (3)	0.36568 (14)	0.0504 (4)
H3	0.0516 (14)	1.306 (2)	0.3220 (13)	0.0494 (5)*
C1	0.0580 (2)	1.1684 (4)	0.1886 (2)	0.0372 (7)
C2	0.0943 (2)	1.0716 (5)	0.2953 (2)	0.0456 (5)
C3	0.0175 (2)	0.8989 (5)	0.2980 (2)	0.0427 (8)
C4	−0.0720 (2)	0.8274 (5)	0.2139 (3)	0.0551 (10)
H4	−0.0888	0.8849	0.1501	0.066*
C5	−0.1370 (3)	0.6698 (6)	0.2241 (3)	0.0744 (12)
H5	−0.1967	0.6208	0.1671	0.089*
C6	−0.1138 (3)	0.5862 (7)	0.3177 (3)	0.0817 (12)
H6	−0.1577	0.4807	0.3241	0.098*
C7	−0.0272 (3)	0.6567 (6)	0.4007 (3)	0.0767 (11)
H7	−0.0116	0.5995	0.4643	0.092*
C8	0.0380 (2)	0.8128 (5)	0.3916 (2)	0.0557 (9)
H8	0.0969	0.8612	0.4496	0.067*
C9	0.2128 (2)	0.9993 (5)	0.32753 (19)	0.0387 (8)
C10	0.2426 (2)	0.7957 (5)	0.3236 (2)	0.0432 (8)

H10	0.1885	0.6938	0.3033	0.052*
C11	0.3508 (2)	0.7417 (6)	0.3492 (2)	0.0549 (9)
H11	0.3694	0.6039	0.3473	0.066*
C12	0.4309 (3)	0.8897 (6)	0.3772 (2)	0.0637 (11)
H12	0.5037	0.8538	0.3926	0.076*
C13	0.4033 (3)	1.0900 (6)	0.3823 (3)	0.0747 (12)
H13	0.4579	1.1911	0.4022	0.090*
C14	0.2957 (3)	1.1449 (6)	0.3584 (3)	0.0666 (11)
H14	0.2786	1.2826	0.3632	0.080*
C15	0.5325 (3)	0.5414 (7)	0.1174 (3)	0.0720 (12)
H15A	0.5331	0.4874	0.0550	0.086*
H15B	0.5704	0.6733	0.1315	0.086*
C16	0.5942 (2)	0.3939 (6)	0.2040 (2)	0.0518 (9)
C17	0.6351 (3)	0.2125 (6)	0.1885 (2)	0.0648 (11)
H17	0.6273	0.1796	0.1232	0.078*
C18	0.6881 (3)	0.0748 (6)	0.2670 (3)	0.0748 (12)
H18	0.7166	−0.0474	0.2542	0.090*
C19	0.6987 (3)	0.1173 (7)	0.3634 (3)	0.0815 (6)
C20	0.6607 (2)	0.3063 (7)	0.3806 (2)	0.0693 (12)
H20	0.6708	0.3423	0.4462	0.083*
C21	0.6089 (3)	0.4393 (6)	0.3022 (3)	0.0613 (11)
H21	0.5826	0.5640	0.3151	0.074*
C22	0.4140 (2)	0.5740 (6)	0.1020 (2)	0.0548 (9)
C23	0.3468 (3)	0.4093 (6)	0.0959 (3)	0.0828 (14)
H23	0.3743	0.2764	0.0984	0.099*
C24	0.2398 (3)	0.4332 (5)	0.0861 (3)	0.0735 (14)
H24	0.1962	0.3188	0.0824	0.088*
C25	0.1999 (2)	0.6279 (4)	0.0821 (2)	0.0410 (8)
C26	0.2638 (3)	0.7928 (5)	0.0868 (3)	0.0631 (10)
H26	0.2359	0.9256	0.0834	0.076*
C27	0.3705 (3)	0.7642 (6)	0.0967 (3)	0.0634 (10)
H27	0.4136	0.8792	0.0998	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0838 (5)	0.0846 (5)	0.0840 (5)	−0.0006 (5)	0.0320 (5)	0.0028 (5)
N2	0.0431 (12)	0.0351 (12)	0.0406 (12)	0.0053 (11)	0.0092 (10)	0.0012 (11)
O1	0.0542 (10)	0.0411 (11)	0.0327 (9)	0.0047 (10)	0.0125 (8)	−0.0027 (9)
O2	0.0853 (13)	0.0403 (12)	0.0712 (11)	0.0183 (11)	0.0466 (10)	0.0154 (10)
O3	0.0534 (5)	0.0472 (5)	0.0485 (5)	0.0033 (5)	0.0192 (5)	−0.0058 (5)
C1	0.0332 (13)	0.0301 (14)	0.0467 (14)	0.0003 (12)	0.0152 (11)	0.0005 (12)
C2	0.0499 (7)	0.0436 (8)	0.0448 (7)	0.0030 (7)	0.0211 (7)	−0.0065 (7)
C3	0.0392 (13)	0.0397 (16)	0.0556 (15)	0.0073 (12)	0.0261 (11)	−0.0027 (13)
C4	0.0417 (15)	0.055 (2)	0.0672 (18)	−0.0041 (15)	0.0218 (14)	−0.0059 (16)
C5	0.0455 (16)	0.075 (3)	0.105 (3)	−0.0162 (19)	0.0339 (17)	−0.013 (2)
C6	0.0689 (18)	0.065 (2)	0.133 (3)	0.0030 (19)	0.0631 (17)	0.013 (2)
C7	0.0730 (18)	0.078 (2)	0.101 (2)	0.017 (2)	0.0582 (16)	0.037 (2)

C8	0.0512 (15)	0.060 (2)	0.0647 (17)	0.0075 (16)	0.0331 (13)	0.0121 (16)
C9	0.0389 (14)	0.0387 (15)	0.0324 (13)	−0.0027 (12)	0.0090 (11)	−0.0054 (12)
C10	0.0408 (14)	0.0454 (18)	0.0403 (13)	−0.0015 (14)	0.0141 (11)	−0.0046 (13)
C11	0.0496 (16)	0.0562 (19)	0.0561 (16)	0.0145 (16)	0.0195 (13)	0.0075 (17)
C12	0.0366 (16)	0.080 (3)	0.065 (2)	0.0069 (18)	0.0122 (15)	−0.0075 (19)
C13	0.0450 (17)	0.071 (2)	0.099 (3)	−0.0225 (18)	0.0217 (17)	−0.021 (2)
C14	0.0548 (18)	0.050 (2)	0.090 (2)	−0.0086 (17)	0.0255 (17)	−0.0165 (18)
C15	0.0590 (18)	0.078 (2)	0.079 (2)	0.0088 (19)	0.0286 (16)	0.026 (2)
C16	0.0382 (14)	0.069 (2)	0.0492 (16)	0.0012 (16)	0.0192 (12)	0.0042 (16)
C17	0.0620 (18)	0.080 (3)	0.0461 (16)	0.0125 (19)	0.0168 (15)	−0.0044 (18)
C18	0.069 (2)	0.064 (2)	0.083 (2)	0.0182 (19)	0.0236 (18)	−0.003 (2)
C19	0.0796 (8)	0.0830 (8)	0.0803 (8)	−0.0017 (8)	0.0320 (8)	0.0049 (8)
C20	0.0512 (18)	0.109 (3)	0.0409 (15)	−0.006 (2)	0.0120 (14)	−0.0057 (18)
C21	0.0473 (16)	0.073 (2)	0.0655 (19)	−0.0008 (17)	0.0260 (14)	−0.0143 (18)
C22	0.0481 (15)	0.056 (2)	0.0562 (17)	0.0061 (16)	0.0179 (13)	0.0106 (17)
C23	0.058 (2)	0.050 (2)	0.128 (3)	0.0112 (18)	0.026 (2)	0.008 (2)
C24	0.0470 (18)	0.0326 (17)	0.128 (3)	0.0000 (15)	0.024 (2)	0.000 (2)
C25	0.0429 (14)	0.0386 (16)	0.0339 (13)	0.0050 (13)	0.0087 (12)	0.0013 (12)
C26	0.0788 (19)	0.0389 (18)	0.088 (2)	0.0061 (17)	0.0508 (16)	0.0031 (16)
C27	0.0634 (17)	0.0506 (19)	0.093 (2)	−0.0058 (17)	0.0494 (15)	0.0045 (18)

Geometric parameters (Å, °)

N1—C19	1.416 (5)	C11—H11	0.9300
N1—H1A	0.872 (10)	C12—C13	1.359 (6)
N1—H1B	0.870 (10)	C12—H12	0.9300
N2—C25	1.458 (4)	C13—C14	1.375 (5)
N2—H2A	0.904 (9)	C13—H13	0.9300
N2—H2B	0.903 (9)	C14—H14	0.9300
N2—H2C	0.905 (10)	C15—C16	1.514 (5)
O1—C1	1.249 (3)	C15—C22	1.515 (5)
O2—C1	1.251 (3)	C15—H15A	0.9700
O3—C2	1.432 (4)	C15—H15B	0.9700
O3—H3	0.827 (9)	C16—C17	1.353 (5)
C1—C2	1.542 (4)	C16—C21	1.381 (5)
C2—C9	1.522 (4)	C17—C18	1.382 (5)
C2—C3	1.528 (4)	C17—H17	0.9300
C3—C8	1.381 (4)	C18—C19	1.368 (6)
C3—C4	1.379 (4)	C18—H18	0.9300
C4—C5	1.387 (5)	C19—C20	1.386 (6)
C4—H4	0.9300	C20—C21	1.359 (5)
C5—C6	1.366 (6)	C20—H20	0.9300
C5—H5	0.9300	C21—H21	0.9300
C6—C7	1.349 (5)	C22—C27	1.350 (5)
C6—H6	0.9300	C22—C23	1.372 (5)
C7—C8	1.375 (5)	C23—C24	1.382 (5)
C7—H7	0.9300	C23—H23	0.9300
C8—H8	0.9300	C24—C25	1.361 (4)
C9—C14	1.378 (4)	C24—H24	0.9300

C9—C10	1.385 (4)	C25—C26	1.350 (4)
C10—C11	1.376 (4)	C26—C27	1.382 (5)
C10—H10	0.9300	C26—H26	0.9300
C11—C12	1.364 (5)	C27—H27	0.9300
C19—N1—H1A	99.2 (14)	C12—C13—C14	120.7 (3)
C19—N1—H1B	98.5 (15)	C12—C13—H13	119.6
H1A—N1—H1B	161.9 (19)	C14—C13—H13	119.6
C25—N2—H2A	112.6 (12)	C9—C14—C13	121.0 (3)
C25—N2—H2B	114.1 (15)	C9—C14—H14	119.5
H2A—N2—H2B	107 (2)	C13—C14—H14	119.5
C25—N2—H2C	112.0 (12)	C16—C15—C22	112.4 (3)
H2A—N2—H2C	108.2 (18)	C16—C15—H15A	109.1
H2B—N2—H2C	102 (2)	C22—C15—H15A	109.1
C2—O3—H3	95.4 (14)	C16—C15—H15B	109.1
O2—C1—O1	124.4 (3)	C22—C15—H15B	109.1
O2—C1—C2	116.8 (3)	H15A—C15—H15B	107.9
O1—C1—C2	118.8 (2)	C17—C16—C21	117.4 (3)
O3—C2—C9	107.4 (2)	C17—C16—C15	121.9 (3)
O3—C2—C3	108.0 (2)	C21—C16—C15	120.6 (3)
C9—C2—C3	112.8 (2)	C16—C17—C18	121.9 (3)
O3—C2—C1	109.1 (2)	C16—C17—H17	119.0
C9—C2—C1	106.4 (2)	C18—C17—H17	119.0
C3—C2—C1	113.0 (2)	C19—C18—C17	120.3 (4)
C8—C3—C4	118.1 (3)	C19—C18—H18	119.8
C8—C3—C2	117.4 (2)	C17—C18—H18	119.8
C4—C3—C2	124.4 (3)	C18—C19—C20	118.0 (4)
C3—C4—C5	120.1 (3)	C18—C19—N1	121.0 (4)
C3—C4—H4	119.9	C20—C19—N1	120.9 (4)
C5—C4—H4	119.9	C21—C20—C19	120.5 (3)
C6—C5—C4	120.3 (3)	C21—C20—H20	119.8
C6—C5—H5	119.8	C19—C20—H20	119.8
C4—C5—H5	119.8	C20—C21—C16	121.7 (4)
C7—C6—C5	120.0 (4)	C20—C21—H21	119.1
C7—C6—H6	120.0	C16—C21—H21	119.1
C5—C6—H6	120.0	C27—C22—C23	116.9 (3)
C6—C7—C8	120.3 (4)	C27—C22—C15	122.2 (3)
C6—C7—H7	119.9	C23—C22—C15	120.9 (3)
C8—C7—H7	119.9	C22—C23—C24	122.5 (3)
C7—C8—C3	121.1 (3)	C22—C23—H23	118.7
C7—C8—H8	119.5	C24—C23—H23	118.7
C3—C8—H8	119.5	C25—C24—C23	118.5 (3)
C14—C9—C10	117.4 (3)	C25—C24—H24	120.7
C14—C9—C2	118.5 (3)	C23—C24—H24	120.7
C10—C9—C2	124.0 (3)	C26—C25—C24	120.2 (3)
C11—C10—C9	121.2 (3)	C26—C25—N2	120.9 (3)
C11—C10—H10	119.4	C24—C25—N2	118.9 (3)
C9—C10—H10	119.4	C25—C26—C27	120.0 (3)
C12—C11—C10	120.2 (3)	C25—C26—H26	120.0
C12—C11—H11	119.9	C27—C26—H26	120.0

C10—C11—H11	119.9	C22—C27—C26	121.8 (3)
C11—C12—C13	119.4 (3)	C22—C27—H27	119.1
C11—C12—H12	120.3	C26—C27—H27	119.1
C13—C12—H12	120.3		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.827 (9)	1.984 (19)	2.586 (3)	129 (2)
N2—H2C···O2^{i}	0.905 (10)	1.851 (11)	2.756 (3)	177.5 (18)
N2—H2B···O1^{ii}	0.903 (9)	1.818 (11)	2.711 (3)	170 (3)
N2—H2A···O1	0.904 (9)	1.865 (9)	2.759 (3)	169.6 (19)

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

Fig. 1

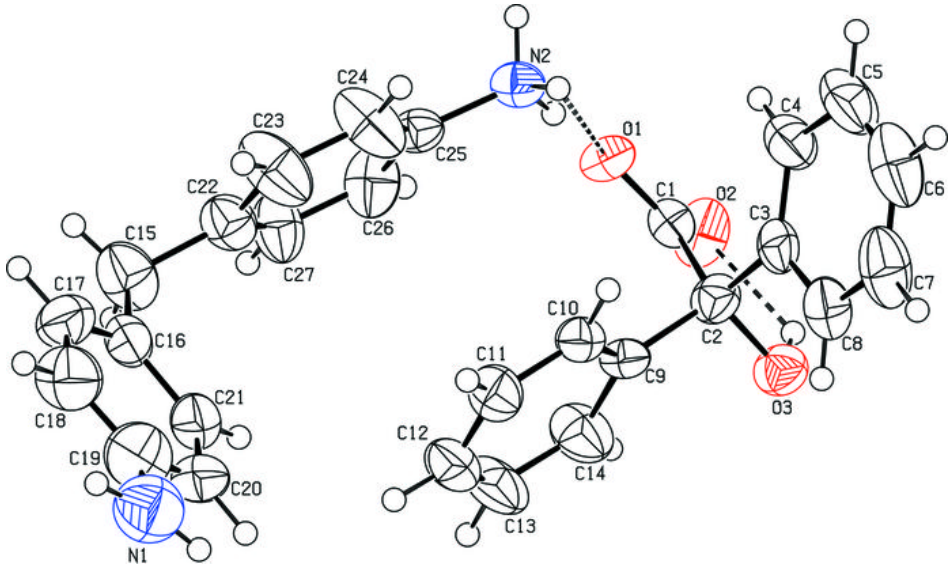
N2
C24
C23
C25
O1
C5
C4
C22
C1
O2
C6
C3
C15
C26
C27
C17
C10
C7
C16
C2
C8
C11
C9
C21
O3
C18
C12
C14
C19
C20
C13
N1

Fig. 2