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3-[(*Z*)-(4-Diethylamino-6-oxocyclohexa-2,4-dien-1-ylidene)methylamino]benzoic acid

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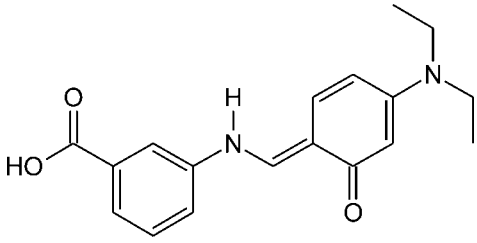
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.124; data-to-parameter ratio = 12.4.

The title compound, $C_{18}H_{20}N_2O_3$, crystallizes as the keto tautomer, unlike the vast majority of similar structures that have been reported that contain the hydroxy tautomer. There are two strong hydrogen bonds in the crystal structure, both accepted by the same carbonyl group: one intramolecular N—H···O and one intermolecular O—H···O. As a result, the carbonyl C=O distance is long, at 1.310 (2) Å, which may suggest the molecule has a significant zwitterionic character. The dihedral angle between the benzene ring planes is 15.05 (7)°. As a result of the intramolecular hydrogen bond, the bridging C—C=N—C group is almost coplanar with the benzene ring that has the diethylamino substituent [dihedral angle 2.35 (15)°].

Related literature

For related structures, see: Büyükgüngör *et al.* (2007); Odabaşoğlu *et al.* (2007); Yathirajan *et al.* (2007). For biological applications, see Hodnett & Dunn (1970); Misra *et al.* (1981); Agarwal *et al.* (1983); Varma *et al.* (1986); Singh & Dash (1988). For related literature, see: Allen (2002).



Experimental

Crystal data

$C_{18}H_{20}N_2O_3$
M_r = 312.36
Monoclinic, $P2_1/n$
a = 9.0904 (13) Å
b = 9.8993 (9) Å
c = 17.8208 (19) Å
β = 100.068 (2)°
V = 1579.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (1) K
0.3 × 0.2 × 0.2 mm

Data collection

KUMA KM4CCD diffractometer
Absorption correction: none
12993 measured reflections
3514 independent reflections
2464 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.124
S = 0.98
3514 reflections
283 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7···O10	0.91 (2)	1.81 (2)	2.578 (2)	140 (2)
O1*A*2—H1*A*2···O10^{i}	1.07 (3)	1.40 (3)	2.467 (1)	173 (2)
C5—H5···O1*A*1^{ii}	0.98 (2)	2.48 (2)	3.449 (2)	174 (2)
C8—H8···O1*A*1^{iii}	0.96 (2)	2.63 (2)	3.436 (2)	142 (1)
C11—H11···O1*A*2^{iv}	0.98 (2)	2.60 (2)	3.244 (2)	124 (1)
C16—H16*A*···O1*A*1^{v}	1.00 (2)	2.60 (2)	3.570 (2)	163 (1)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+\frac{5}{2}, y+\frac{1}{2}, -z+\frac{5}{2}$; (iii) $-x+2, -y, -z+2$; (iv) $x, y+1, z$; (v) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1989); software used to prepare material for publication: *SHELXL97*and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2063).

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supplementary materials

Acta Cryst. (2008). E**64**, o163-o164 [**doi:10.1107/S1600536807064446**]

3-[(*Z*)-(4-Diethylamino-6-oxocyclohexa-2,4-dien-1-ylidene)methylamino]benzoic acid

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Comment

Schiff bases are used as substrates in the preparation of number of industrial and biologically active compounds *via* ring closure, cycloaddition and replacement reactions. Some Schiff base derivatives were reported to possess antimicrobial, anti-inflammatory and central nervous system activities. Moreover, Schiff bases are also known to have biological activities such as antimicrobial, antifungal, antitumor and as herbicides (*e.g.* Hodnett *et al.*, 1970, Singh & Dash, 1988, Varma *et al.*, (1986)). In the course of our studies of Schiff bases (*e.g.* Büyükgüngör *et al.*, 2007; Odabaşoğlu *et al.*, 2007; Yathirajan *et al.*, 2007), the title compound, $C_{18}H_{20}N_2O_3$ was synthesized and its crystal structure is reported.

The title compound crystallizes as the keto-tautomer (Fig. 1), unlike the majority of the similar compounds. In the CSD (Allen, 2002) the hydroxy tautomers were found in 218 compounds while the keto ones only in 17 compounds (Version Nov. 2006, updates up to August 2007; only organic compounds). In this case the presence of the certain tautomer is proven by the succesful location and refinement of the hydrogen atom bonded to N7 nitrogen atom (Fig. 2a). Short and relatively linear intramolecular N—H···O hydrogen bond forms an almost planar (maximum deviation 0.017 (1) Å) six-membered ring. The same O10 oxygen atom which accepts the intramolecular hydrogen bond is involved in a very short (O···O distance is 2.467 (1) Å) intermolecular O—H···O hydrogen bond. As a result the C10—O10 bond of 1.310 (2)Å is significantly longer than a typical C═O double bond. CSD search results show that such elongation is typical for similar compounds, the mean C—O distance being 1.348 (17)Å for hydroxy tautomers, but it may also be as large as 1.299 (17)Å also for the keto-tautomers. Together with the observation of bond lengths around N7 atom this implies some degree of zwitterionic character of the molecule, with partial positive charge at N7—H7 group and negative at O10 atom. These perturbations disturb also the benzene ring. The ring A (C1 - C6) is closer to planarity than the ring B (C9 - C14). Maximum deviations from the least-squares planes are 0.0103 (11)Å for ring A and 0.0219 (12)Å for ring B. Also the bond lengths and angles are much more uniform within the ring A than in ring B.

The conformation of the molecule is described by the dihedral angles between benzene ring planes of 15.05 (7)°. As a result of the intramolecular hydrogen bond, the bridging C—C═N—C group is almost coplanar with the ring B (dihedral angle 2.35 (15)°). The COO group is significantly, by 21.73 (10)°, twisted with respect to its parent ring's plane. On the other end of the molecule, the C—N—C fragment is twisted by 17.0 (2)°, while the terminal C—C bonds are almost perpendicular to the CNC plane.

In the crystal structure the molecules are connected by strong intermolecular O—H···O hydrogen bonds into tapes along the *y*-direction. The O—H bond is significantly elongated, to 1.07 (3)Å due to the formation of the hydrogen bond (*cf.* Fig. 2 b). The tapes are connected by relatively strong inter-tape C—H···O hydrogen bonds into the layers (Fig. 3). Some additional C—H···O interactions (Table 1) also play a role in the building of the crystal structure.

Experimental

A mixture of 3-aminobenzoic acid (1.37 g, 0.01 mol) and 4-(diethylamino)-2-hydroxybenzaldehyde (1.92 g, 0.01 mol) in 25 ml of absolute ethanol containing 2 drops of 4 *M* sulfuric acid was refluxed for about 5 h. On cooling, the separated solid was filtered and recrystallized from DMF (m.p.: 483–485 K). The expected product was 3-({(1E)-[4-(diethylamino)-2-hydroxyphenyl]methylene}amino)benzoic acid, but the obtained product was the tautomeric form 3-({(*Z*)-[4-(diethylamino)-6-oxocyclohexa-2,4-dien-1-ylidene]methyl} amino)benzoic acid. Analysis for $C_{18}H_{20}N_2O_3$: Found (Calculated): C: 69.12 (69.21); H: 6.38 (6.45); N: 8.90% (8.97%).

Refinement

The hydrogen atoms were located in the difference Fourier maps and refined as 'riding model'. Isotropic displacement parameters for hydrogen atoms were set at 1.2 (1.3 for methyl group) times the U_{eq} values of appropriate carrier atoms.

Figures

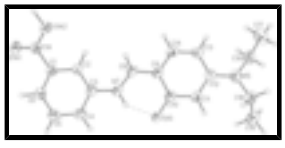

Fig. 1. Anisotropic displacement ellipsoids representation (50% probability level) of the molecule with the atom labelling scheme, iIntramolecular hydrogen bond is depicted in dashed line.

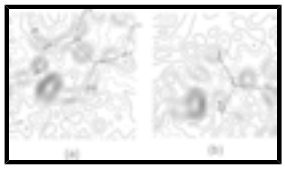

Fig. 2. Difference Fourier map slices calculated for a model without the hydrogen atoms involved in intramolecular hydrogen bonds: (*a*) H7, (*b*) H1A2 (Farrugia, 1999). Solid lines: positive values, dashed: negative; contour level: 0.04 e\%A^-3^.

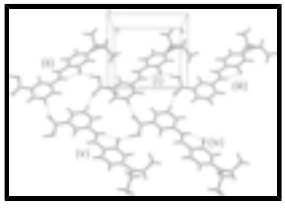

Fig. 3. The hydrogen-bonded layer as seen approximately along the *c* axis. Symmetry codes: (i) *x*,*y*,*z* (ii) *x*,-1 + *y*,*z* (iii) *x*,1 + *y*,*z* (iv) 5/2 − *x*,1/2 + *y*,5/2 − *z* (v) 5/2 − *x*,-1/2 + *y*,5/2 − *z*.

3-[(*Z*)-(4-Diethylamino-6-oxocyclohexa-2,4-dien-1- ylidene)methylamino]benzoic acid

Crystal data

$C_{18}H_{20}N_2O_3$	F_{000} = 664
M_r = 312.36	D_x = 1.314 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5056 reflections
a = 9.0904 (13) Å	θ = 3–24º
b = 9.8993 (9) Å	μ = 0.09 mm^{-1}
c = 17.8208 (19) Å	*T* = 295 (1) K
β = 100.068 (2)º	Block, purple

V = 1579.0 (3) Å^3
Z = 4

0.3 × 0.2 × 0.2 mm

Data collection

KUMA KM4CCD four-circle diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 8.1929 pixels mm^{-1}
T = 293(2) K
ω scan
Absorption correction: none
12993 measured reflections

3514 independent reflections
2464 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 28.0º
θ_{min} = 2.4º
h = −11→11
k = −12→12
l = −23→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.124
S = 0.98
3514 reflections
283 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 0.4649P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0026 (8)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.03151 (16)	0.06899 (14)	1.12525 (8)	0.0326 (3)
C1A	1.00497 (17)	−0.07858 (14)	1.10991 (8)	0.0353 (3)
O1A1	1.09883 (14)	−0.16365 (11)	1.13287 (7)	0.0535 (3)
O1A2	0.87299 (13)	−0.10532 (11)	1.07198 (7)	0.0509 (3)
H1A2	0.850 (3)	−0.211 (3)	1.0667 (14)	0.098 (8)*
C2	0.94453 (17)	0.16506 (14)	1.08096 (8)	0.0330 (3)
H2	0.8663 (17)	0.1354 (16)	1.0377 (9)	0.035 (4)*
C3	0.96859 (17)	0.30147 (14)	1.09759 (8)	0.0347 (3)
C4	1.07595 (18)	0.34076 (15)	1.15860 (9)	0.0401 (4)
H4	1.0907 (18)	0.4382 (18)	1.1696 (9)	0.043 (4)*
C5	1.16149 (19)	0.24488 (17)	1.20297 (9)	0.0432 (4)
H5	1.234 (2)	0.2745 (18)	1.2469 (10)	0.050 (5)*
C6	1.14098 (17)	0.10890 (16)	1.18570 (9)	0.0388 (3)

H6	1.2029 (19)	0.0408 (19)	1.2189 (10)	0.048 (5)*
N7	0.88185 (16)	0.40373 (12)	1.05574 (7)	0.0401 (3)
H7	0.887 (2)	0.489 (2)	1.0747 (11)	0.065 (6)*
C8	0.78879 (19)	0.39282 (15)	0.99049 (9)	0.0411 (4)
H8	0.7807 (19)	0.3078 (19)	0.9646 (10)	0.051 (5)*
C9	0.70296 (19)	0.49992 (14)	0.95604 (9)	0.0398 (4)
C10	0.71045 (18)	0.63293 (14)	0.99024 (8)	0.0372 (3)
O10	0.80433 (15)	0.65435 (10)	1.05372 (6)	0.0485 (3)
C11	0.62075 (19)	0.73538 (15)	0.95329 (9)	0.0392 (4)
H11	0.6353 (18)	0.8253 (17)	0.9767 (9)	0.041 (4)*
C12	0.53163 (17)	0.71697 (15)	0.88196 (9)	0.0388 (4)
C13	0.5272 (2)	0.58514 (17)	0.84767 (10)	0.0482 (4)
H13	0.466 (2)	0.5678 (18)	0.7969 (11)	0.054 (5)*
C14	0.6085 (2)	0.48282 (16)	0.88451 (10)	0.0482 (4)
H14	0.602 (2)	0.392 (2)	0.8607 (10)	0.059 (5)*
N15	0.45111 (16)	0.82021 (13)	0.84509 (8)	0.0449 (3)
C16	0.3912 (2)	0.8173 (2)	0.76261 (10)	0.0495 (4)
H16A	0.457 (2)	0.7599 (18)	0.7356 (10)	0.054 (4)*
H16B	0.394 (2)	0.908 (2)	0.7398 (10)	0.054 (4)*
C17	0.2318 (2)	0.7704 (3)	0.74366 (13)	0.0670 (6)
H17A	0.228 (3)	0.675 (3)	0.7658 (15)	0.098 (5)*
H17B	0.200 (3)	0.773 (3)	0.6867 (16)	0.098 (5)*
H17C	0.161 (3)	0.833 (3)	0.7715 (15)	0.098 (5)*
C18	0.4280 (2)	0.94628 (17)	0.88460 (10)	0.0442 (4)
H18A	0.4192 (18)	0.9237 (17)	0.9378 (10)	0.045 (3)*
H18B	0.334 (2)	0.9777 (17)	0.8604 (10)	0.045 (3)*
C19	0.5467 (2)	1.05246 (19)	0.88190 (13)	0.0552 (5)
H19A	0.647 (2)	1.021 (2)	0.9066 (12)	0.071 (4)*
H19B	0.523 (2)	1.138 (2)	0.9093 (12)	0.071 (4)*
H19C	0.549 (2)	1.075 (2)	0.8283 (13)	0.071 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0348 (8)	0.0296 (7)	0.0333 (7)	0.0018 (6)	0.0059 (6)	0.0005 (6)
C1A	0.0403 (8)	0.0294 (7)	0.0354 (7)	0.0035 (6)	0.0047 (6)	0.0014 (6)
O1A1	0.0530 (7)	0.0334 (6)	0.0680 (8)	0.0117 (5)	−0.0068 (6)	0.0036 (5)
O1A2	0.0482 (7)	0.0247 (6)	0.0722 (8)	0.0033 (5)	−0.0105 (6)	−0.0060 (5)
C2	0.0366 (8)	0.0272 (7)	0.0338 (7)	−0.0008 (6)	0.0021 (6)	−0.0013 (5)
C3	0.0417 (8)	0.0271 (7)	0.0361 (7)	−0.0003 (6)	0.0090 (6)	0.0001 (6)
C4	0.0453 (9)	0.0298 (8)	0.0445 (9)	−0.0059 (6)	0.0061 (7)	−0.0067 (6)
C5	0.0408 (9)	0.0453 (9)	0.0410 (9)	−0.0053 (7)	0.0001 (7)	−0.0081 (7)
C6	0.0365 (8)	0.0386 (8)	0.0395 (8)	0.0031 (7)	0.0017 (6)	0.0005 (6)
N7	0.0538 (8)	0.0219 (6)	0.0418 (7)	0.0012 (6)	0.0009 (6)	0.0000 (5)
C8	0.0562 (10)	0.0224 (7)	0.0436 (8)	−0.0012 (7)	0.0053 (7)	−0.0022 (6)
C9	0.0525 (9)	0.0240 (7)	0.0405 (8)	−0.0010 (7)	0.0020 (7)	−0.0010 (6)
C10	0.0470 (9)	0.0256 (7)	0.0371 (8)	−0.0022 (6)	0.0022 (7)	−0.0021 (6)
O10	0.0707 (8)	0.0234 (5)	0.0433 (6)	0.0011 (5)	−0.0131 (6)	−0.0034 (4)

C11	0.0502 (9)	0.0243 (7)	0.0407 (8)	0.0022 (6)	0.0009 (7)	−0.0047 (6)
C12	0.0407 (9)	0.0317 (7)	0.0423 (8)	0.0012 (6)	0.0021 (7)	−0.0018 (6)
C13	0.0555 (11)	0.0379 (9)	0.0449 (9)	−0.0005 (8)	−0.0087 (8)	−0.0082 (7)
C14	0.0636 (11)	0.0276 (8)	0.0489 (9)	−0.0003 (7)	−0.0026 (8)	−0.0076 (7)
N15	0.0495 (8)	0.0375 (7)	0.0436 (7)	0.0080 (6)	−0.0031 (6)	−0.0014 (6)
C16	0.0528 (11)	0.0497 (10)	0.0452 (9)	0.0063 (8)	0.0059 (8)	0.0031 (8)
C17	0.0530 (12)	0.0885 (17)	0.0554 (12)	0.0000 (11)	−0.0018 (10)	−0.0032 (11)
C18	0.0447 (10)	0.0390 (8)	0.0480 (9)	0.0116 (7)	0.0058 (8)	0.0012 (7)
C19	0.0618 (12)	0.0410 (10)	0.0636 (12)	0.0016 (9)	0.0128 (10)	−0.0003 (9)

Geometric parameters (Å, °)

C1—C6	1.390 (2)	C10—C11	1.393 (2)
C1—C2	1.391 (2)	C11—C12	1.395 (2)
C1—C1A	1.498 (2)	C11—H11	0.982 (17)
C1A—O1A1	1.2177 (18)	C12—N15	1.3578 (19)
C1A—O1A2	1.2972 (19)	C12—C13	1.439 (2)
O1A2—H1A2	1.07 (3)	C13—C14	1.354 (2)
C2—C3	1.392 (2)	C13—H13	0.991 (18)
C2—H2	0.998 (16)	C14—H14	1.00 (2)
C3—C4	1.384 (2)	N15—C18	1.466 (2)
C3—N7	1.4132 (19)	N15—C16	1.476 (2)
C4—C5	1.384 (2)	C16—C17	1.503 (3)
C4—H4	0.989 (17)	C16—H16A	1.004 (19)
C5—C6	1.386 (2)	C16—H16B	0.990 (19)
C5—H5	0.975 (18)	C17—H17A	1.03 (3)
C6—H6	1.002 (18)	C17—H17B	1.01 (3)
N7—C8	1.317 (2)	C17—H17C	1.07 (3)
N7—H7	0.91 (2)	C18—C19	1.513 (3)
C8—C9	1.394 (2)	C18—H18A	0.990 (18)
C8—H8	0.956 (19)	C18—H18B	0.942 (18)
C9—C14	1.417 (2)	C19—H19A	0.99 (2)
C9—C10	1.448 (2)	C19—H19B	1.02 (2)
C10—O10	1.3097 (18)	C19—H19C	0.99 (2)
C6—C1—C2	120.30 (13)	N15—C12—C11	121.38 (14)
C6—C1—C1A	119.30 (13)	N15—C12—C13	120.31 (14)
C2—C1—C1A	120.38 (13)	C11—C12—C13	118.31 (14)
O1A1—C1A—O1A2	124.32 (14)	C14—C13—C12	120.03 (15)
O1A1—C1A—C1	122.15 (14)	C14—C13—H13	119.0 (11)
O1A2—C1A—C1	113.51 (13)	C12—C13—H13	120.9 (11)
C1A—O1A2—H1A2	113.4 (13)	C13—C14—C9	122.70 (15)
C1—C2—C3	119.34 (14)	C13—C14—H14	119.1 (11)
C1—C2—H2	119.7 (9)	C9—C14—H14	118.2 (11)
C3—C2—H2	121.0 (9)	C12—N15—C18	121.24 (13)
C4—C3—C2	120.21 (14)	C12—N15—C16	122.74 (14)
C4—C3—N7	117.72 (13)	C18—N15—C16	115.87 (13)
C2—C3—N7	122.02 (14)	N15—C16—C17	113.77 (16)
C3—C4—C5	120.31 (14)	N15—C16—H16A	110.0 (10)
C3—C4—H4	118.8 (9)	C17—C16—H16A	110.3 (10)

C5—C4—H4	120.8 (10)	N15—C16—H16B	111.0 (11)
C4—C5—C6	119.92 (15)	C17—C16—H16B	106.3 (11)
C4—C5—H5	119.0 (11)	H16A—C16—H16B	105.0 (15)
C6—C5—H5	121.0 (11)	C16—C17—H17A	106.9 (15)
C5—C6—C1	119.89 (15)	C16—C17—H17B	108.2 (15)
C5—C6—H6	118.8 (10)	H17A—C17—H17B	113 (2)
C1—C6—H6	121.2 (10)	C16—C17—H17C	110.5 (14)
C8—N7—C3	128.32 (13)	H17A—C17—H17C	107 (2)
C8—N7—H7	113.0 (13)	H17B—C17—H17C	112 (2)
C3—N7—H7	118.7 (13)	N15—C18—C19	114.44 (15)
N7—C8—C9	123.38 (14)	N15—C18—H18A	108.1 (10)
N7—C8—H8	118.8 (11)	C19—C18—H18A	111.4 (10)
C9—C8—H8	117.8 (11)	N15—C18—H18B	104.8 (11)
C8—C9—C14	120.66 (14)	C19—C18—H18B	110.6 (11)
C8—C9—C10	121.66 (14)	H18A—C18—H18B	107.1 (14)
C14—C9—C10	117.65 (14)	C18—C19—H19A	111.7 (13)
O10—C10—C11	121.99 (13)	C18—C19—H19B	110.3 (12)
O10—C10—C9	119.11 (13)	H19A—C19—H19B	107.8 (18)
C11—C10—C9	118.86 (14)	C18—C19—H19C	109.2 (13)
C10—C11—C12	122.32 (13)	H19A—C19—H19C	109.2 (17)
C10—C11—H11	115.8 (10)	H19B—C19—H19C	108.5 (17)
C12—C11—H11	121.3 (9)		
C6—C1—C1A—O1A1	−21.1 (2)	C14—C9—C10—O10	−175.35 (15)
C2—C1—C1A—O1A1	160.84 (14)	C8—C9—C10—C11	−179.40 (15)
C6—C1—C1A—O1A2	157.39 (14)	C14—C9—C10—C11	2.7 (2)
C2—C1—C1A—O1A2	−20.7 (2)	O10—C10—C11—C12	173.43 (15)
C6—C1—C2—C3	0.2 (2)	C9—C10—C11—C12	−4.5 (2)
C1A—C1—C2—C3	178.28 (13)	C10—C11—C12—N15	−176.43 (16)
C1—C2—C3—C4	−1.3 (2)	C10—C11—C12—C13	3.3 (3)
C1—C2—C3—N7	−178.63 (13)	N15—C12—C13—C14	179.57 (17)
C2—C3—C4—C5	0.8 (2)	C11—C12—C13—C14	−0.1 (3)
N7—C3—C4—C5	178.23 (14)	C12—C13—C14—C9	−1.6 (3)
C3—C4—C5—C6	0.8 (2)	C8—C9—C14—C13	−177.61 (18)
C4—C5—C6—C1	−1.9 (2)	C10—C9—C14—C13	0.3 (3)
C2—C1—C6—C5	1.4 (2)	C11—C12—N15—C18	−13.4 (2)
C1A—C1—C6—C5	−176.68 (14)	C13—C12—N15—C18	166.90 (16)
C4—C3—N7—C8	170.02 (16)	C11—C12—N15—C16	162.02 (16)
C2—C3—N7—C8	−12.6 (3)	C13—C12—N15—C16	−17.7 (3)
C3—N7—C8—C9	176.68 (15)	C12—N15—C16—C17	95.6 (2)
N7—C8—C9—C14	177.89 (16)	C18—N15—C16—C17	−88.7 (2)
N7—C8—C9—C10	0.0 (3)	C12—N15—C18—C19	89.8 (2)
C8—C9—C10—O10	2.6 (2)	C16—N15—C18—C19	−86.0 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N7—H7···O10	0.91 (2)	1.81 (2)	2.578 (2)	140 (2)
O1A2—H1A2···O10^{i}	1.07 (3)	1.40 (3)	2.467 (1)	173 (2)

C5—H5···O1A1^{ii}	0.98 (2)	2.48 (2)	3.449 (2)	174 (2)
C8—H8···O1A1^{iii}	0.96 (2)	2.63 (2)	3.436 (2)	142 (1)
C11—H11···O1A2^{iv}	0.98 (2)	2.60 (2)	3.244 (2)	124 (1)
C16—H16A···O1A1^{v}	1.00 (2)	2.60 (2)	3.570 (2)	163 (1)

Symmetry codes: (i) x, $y-1$, z; (ii) $-x+5/2$, $y+1/2$, $-z+5/2$; (iii) $-x+2$, $-y$, $-z+2$; (iv) x, $y+1$, z; (v) $x-1/2$, $-y+1/2$, $z-1/2$.

Fig. 1

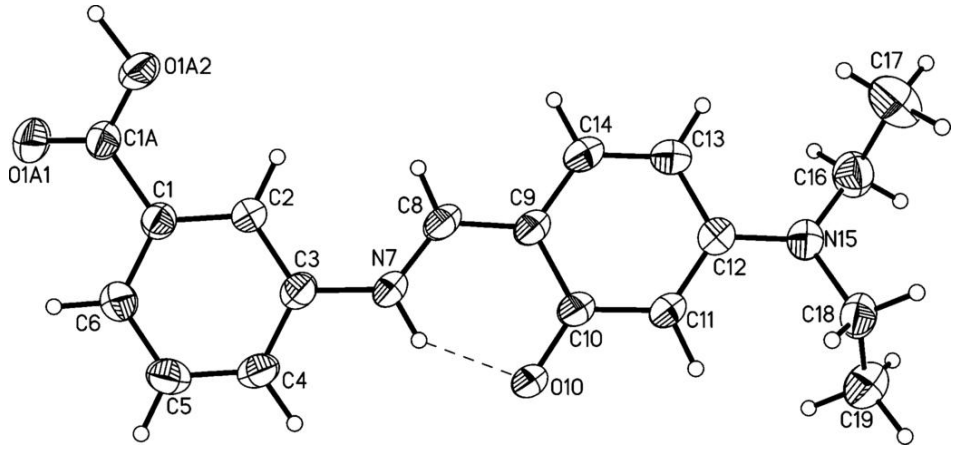
O1A2
C1A
O1A1
C1
C2
C3
N7
C8
C9
C14
C13
C17
C16
N15
C12
C11
C10
O10
C18
C19
C6
C5
C4

Fig. 2

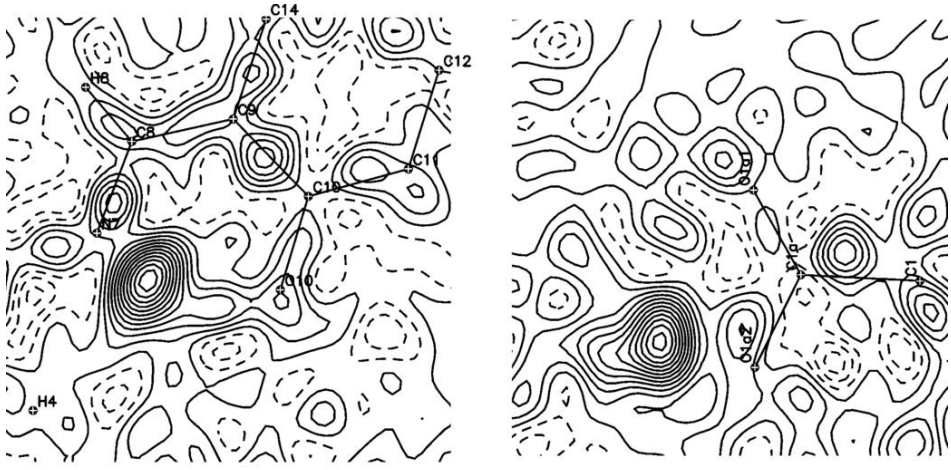

Fig. 3