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2-(2-Hydroxyethyl)-2,3-dihydro-1*H*-benzo[*c*]pyrrol-1-one

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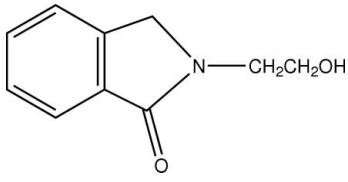
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.039; wR factor = 0.117; data-to-parameter ratio = 16.1.

Two independent molecules, one with slight disorder and unequal distribution of the two –OH components [0.916 (2):0.084 (2)], are present in the title compound, $C_{10}H_{11}NO_2$. The N—CH_2—CH_2—O torsion angles 64.50 (14)° (major component, disordered molecule) and 65.76 (13)° (minor component) are similar. The disordered alcohol groups are symmetrically situated below and above the plane of the imidazole ring atoms. Two types of O—H···O hydrogen bonds are present, forming zigzag chains propagating along the *a*-axis direction. In both cases, the carbonyl O atoms are hydrogen-bond acceptors from the alcohol hydroxy groups, with graph-set motif $C_2^2(14)$ for these O—H···O interactions. There are π–π stacking interactions present, with distances between the substituted pyrrole ring centroids of 3.5317 (6) and 3.6584 (6) Å In addition, C—H···O and C—H···π(arene) interactions are present.

Related literature

For related literature, see: Zuman (2004); Grigg *et al.* (1985); Urban *et al.* (2007). For the biological activity of isoindolines, see: Mukherjee *et al.* (2000).



Experimental

Crystal data

$C_{10}H_{11}NO_2$
M_r = 177.2
Triclinic, $P\overline{1}$
a = 8.7122 (2) Å
b = 9.8523 (2) Å
c = 10.4304 (2) Å
α = 103.2549 (14)°
β = 90.6852 (14)°
γ = 97.4368 (12)°
V = 863.31 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 150 (2) K
0.5 × 0.4 × 0.3 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
25935 measured reflections
3987 independent reflections
3497 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.117
S = 2.09
3987 reflections
248 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Hydrogen bonds and D—H···π-ring interactions from *PLATON* (Spek, 2003).

*Cg*1 and *Cg*2 are the centroids of the rings C2–C7 and C13–C18, respectively.

D—H···A/*Cg*	D—H	H···A/*Cg*	D···A/*Cg*	D—H···A/*Cg*
O2—H2O···O3	0.820 (11)	1.897 (11)	2.7120 (12)	172.1 (13)
O4—H4O···O1^{i}	0.820 (10)	1.947 (10)	2.7636 (11)	173.6 (12)
C6—H6···O2^{ii}	0.93	2.47	3.2590 (14)	143
C16—H16···O2^{iii}	0.93	2.54	3.2171 (14)	130
C20—H20*b*···O3	0.97	2.57	2.9296 (13)	102
C9—H9*a*···*Cg*1^{iv}	0.98	2.97	3.4442 (11)	112
C3—H3···*Cg*2^{v}	0.98	2.92	3.6643 (11)	138
C20—H20*a*···*Cg*2^{vi}	0.98	2.84	3.5668 (12)	132

Symmetry codes: (i) x+1, y, z; (ii) -x+1, -y+1, -z; (iii) x, y-1, z; (iv) -x, -y+1, -z; (v) x-1, y, z; (vi) -x+1, -y+1, -z+1.

Data collection: *COLLECT* (Hooft, 1998) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *COLLECT* and *DENZO*; data reduction: *COLLECT* and *DENZO*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *JANA2000* (Petříček *et al.*, 2000); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *JANA2000*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2022).

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supplementary materials

Acta Cryst. (2007). E**63**, o4137-o4138 [**doi:10.1107/S1600536807045291**]

2-(2-Hydroxyethyl)-2,3-dihydro-1*H*-benzo[*c*]pyrrol-1-one

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Comment

Our research project deals with chemical and electrochemical properties of diketones (Zuman, 2004). As a part of this study, we observed that a main product of the reaction of orthophthalaldehyde with amines in low concentrations about 10^{-3} mol/l is reducible about 0.5 V more negatively than the parent dialdehyde. In order to study this reaction as well as in order to identify the product (an isoindoline derivative is expected to be formed) the reaction of phthalaldehyde with kolamine (2-aminoethanol) was carried out.

In ethanol, however, the reaction results in a mixture of non-separable, viscous, probably polymeric compounds. On the other hand, the reaction in acetonitrile leads to two minor products together with formation of a non-separable mixture. The minor products were isolated, purified, crystallized and analyzed by NMR and single-crystal X-ray diffraction.

One of these compounds was identified as 2-(2-hydroxyetyl)-1H,3H benzo[*c*]pyrrol-1-one, (I), that is here reported while the second compound was identified as (3*R**,1'*S**,3'*R**)-2-(2''-hydroxyethyl)-3- (3'-hydroxy-1'*H*,3'*H*- benzo[*c*]furan)-1'-yl-1*H*,3*H*-benzo[*c*]pyrrol-1-one, (II), (Urban *et al.*, 2007).

The dihedral angles between the pyrrole and the attached phenyl rings in the isoindoline rings are 0.47 (4) and 0.94 (4)° for the moieties containing N1 and N2 atoms, respectively.

The reaction pathways are clearly affected by concentrations of the components and by the composition of the reaction solvent, several simultaneous reactions seem to occur.

The formation of the title compound (I) in acetonitrile proceeds most probably *via* an intramolecular Cannizzaro reaction simultaneously with the addition of kolamine and cyclization. In the case od the second compound (Urban *et al.*, 2007), acyloin condensation of two molecules takes place, followed by acetalization on one ring, whereas the second one undergoes a reaction analogous to the formation the title compound. Since these two isolated compounds are minor products, the main reaction pathway should be different. Its further investigation is currently being performed.

A referee pointed that there may also be an alternative way of preparation of the title compound (I) following Grigg *et al.* (1985). This other way was confirmed experimentally: 500 mg of phthalaldehyde and 228 mg of ethanolamine were dissolved in 7 ml of acetic acid. The mixture was refluxed for 10 minutes and then it was evaporated to dryness. The residue was dissolved in ethanol, treated with active coal and filtered. Evaporation and crystallization of the residue from toluene gave the product (318 mg) as colourless crystals.

A crystal from the prepared batch by the latter way was selected and put on a four-circle single-crystal diffractometer. A trial measurement at room temperature confirmed the identity of the sample whose largest size did not exceed 0.3 mm. The lattice parameters at 291 (1) K were determined as: 8.7940 (11), 9.8820 (13), 10.5320 (13) Å, 103.699 (6), 90.394 (8), 96.788 (7)°.

From the lattice parameters at 291 and 150 K it is seen that the unit-cell dimensions are susceptible to thermal expansion.

Final remark: A referee pointed out that many isoindoline derivatives display biological as well as pharmaceutical activity (Mukherjee *et al.*, 2000).

Experimental

2.33 g of phthalaldehyde were dissolved in 120 ml of dry acetonitrile. 1.3 ml of ethanolamine was added dropwise to the mixture while stirring. The mixture was stirred for 4 h and then it was evaporated to dryness under reduced pressure. The residue was chromatographed on a column of silica gel in $CHCl_3$:C_2H_5OH (10%). All reaction steps were performed at room temperature.

At least two products were produced by the reaction. Column chromatography afforded 308 mg of the title compound, (I) 252 mg after its recrystallization from toluene, as well as 256 mg of 2-(2''-hydroxyethyl)-3-(3'-hydroxy-1'*H*,3'*H*-benzo[*c*]furan)-1'-yl- 1H,3*H*-benzo[*c*]pyrrol-1-one, (II), the yield of which was 150 mg after its recrystallization from $CHCl_3$-n-C_6H_{14} (Urban *et al.*, 2007). The major part of a mixture are polymers.

Refinement

In the vicinity of C10 and O2 atoms were maxima on a difference Fourier map (0.40 and 0.80 e $Å^{-3}$, respectively). These maxima were assigned to the disordered C11 and O5 atoms. These atoms have the respective counterparts of C10 and O2. Since the refined occupational parameters of C11 and O5 were so low (0.0840 (15)) the corresponding H atoms were situated into idealized positions with regard to C11 but could not be assigned to O5.

Otherwise all of the H atoms were discernible in the difference Fourier map. All the H atoms were constrained to the riding-hydrogen formalism with $U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso}(H) = 1.2U_{eq}(O)$. The C—H distances were constrained to 0.93 and 0.97 Å for aryl and methylene H atoms, respectively.

The O—H distances were restrained to 0.820 (1) Å while the C11—O5 distances were restrained to 1.400 (1) Å.

The occupational parameters of C10, H10*a*, H10*b*, O2 as well as H2O were set to be equal while each of the occupational parameters of O5 and C11, H11*a* and H11*b* was a complement to 1 of the former occupational parameters. The displacement parameters of the disordered pairs of the atoms O2, O5 and C10, C11 were also constrained to be equal.

Figures

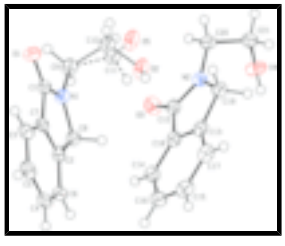

Fig. 1. The title structure (I) with displacement parameters shown at the 50% probability level. The disordered atoms with a lesser occupation are interconnected by dashed lines. H atoms are not included on disordered non-H atoms.

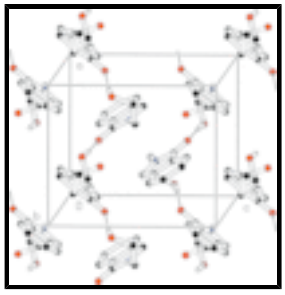

Fig. 2. A view of the title structure (I) with depicted O—H···O hydrogen bonds. The H atoms that are not involved in the O—H···O bonds are not depicted for the sake of clarity.

2-(2-Hydroxyethyl)-2,3-dihydro-1*H*-benzo[*c*]pyrrol-1-one

Crystal data

$C_{10}H_{11}N_1O_2$	$Z = 4$
$M_r = 177.2$	$F_{000} = 375$
Triclinic, $P\bar{1}$	$D_x = 1.363$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.7122$ (2) Å	Cell parameters from 3960 reflections
$b = 9.8523$ (2) Å	$\theta = 1$–27.5º
$c = 10.4304$ (2) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 103.2549$ (14)º	$T = 150$ (2) K
$\beta = 90.6852$ (14)º	Block, colourless
$\gamma = 97.4368$ (12)º	0.5 × 0.4 × 0.3 mm
$V = 863.31$ (3) Å^3	

Data collection

Nonius KappaCCD diffractometer	3987 independent reflections
Radiation source: fine-focus sealed tube	3497 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
Detector resolution: 9.091 pixels mm^{-1}	$\theta_{max} = 27.6$º
$T = 293$ K	$\theta_{min} = 2.0$º
φ and ω scans	$h = -11 \rightarrow 11$
Absorption correction: none	$k = -12 \rightarrow 12$
25935 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	82 constraints
$R[F^2 > 2\sigma(F^2)] = 0.039$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.117$	Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(I) + 0.0016I^2)$
$S = 2.09$	$(\Delta/\sigma)_{max} = 0.006$
3987 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}

248 parameters	$\Delta\rho_{min} = -0.17$ e Å^{-3}
3 restraints	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.09039 (11)	0.54687 (10)	0.19174 (9)	0.0217 (3)	
C2	0.20064 (12)	0.38058 (11)	0.03797 (10)	0.0235 (3)	
C3	0.05043 (12)	0.28378 (10)	0.19853 (10)	0.0266 (3)	
H3	−0.011958	0.2959	0.270909	0.0319*	
C4	0.17827 (13)	0.13502 (11)	0.02850 (11)	0.0325 (4)	
H4	0.201956	0.04596	−0.0109	0.039*	
C5	0.08718 (13)	0.15208 (11)	0.13875 (11)	0.0311 (4)	
H5	0.050678	0.075085	0.172648	0.0374*	
C6	0.23476 (12)	0.24811 (11)	−0.02417 (11)	0.0288 (3)	
H6	0.2936	0.235532	−0.098737	0.0345*	
C7	0.10948 (11)	0.39686 (10)	0.14716 (9)	0.0218 (3)	
C8	0.24652 (12)	0.52148 (10)	0.00785 (10)	0.0247 (3)	
H8a	0.357847	0.547079	0.021077	0.0296*	
H8b	0.20396	0.520935	−0.078651	0.0296*	
C9	0.17687 (12)	0.76534 (10)	0.11899 (10)	0.0267 (3)	
H9a	0.077343	0.795184	0.143598	0.032*	
H9b	0.194941	0.784578	0.032896	0.032*	
C10	0.30195 (14)	0.85174 (13)	0.21711 (13)	0.0268 (4)	0.9162 (15)
H10a	0.295036	0.951035	0.226832	0.0321*	0.9162 (15)
H10b	0.284511	0.831731	0.302999	0.0321*	0.9162 (15)
O1	0.01510 (9)	0.60081 (8)	0.28583 (7)	0.0296 (3)	
O2	0.45202 (10)	0.82422 (9)	0.17828 (10)	0.0357 (3)	0.9162 (15)
H2o	0.4719 (18)	0.7569 (10)	0.2063 (13)	0.0428*	0.9162 (15)
N1	0.16865 (10)	0.61482 (8)	0.10924 (8)	0.0231 (3)	
C12	0.59562 (12)	0.54190 (10)	0.32247 (10)	0.0235 (3)	
C13	0.70896 (12)	0.38520 (11)	0.41794 (10)	0.0237 (3)	
C14	0.56705 (12)	0.27575 (11)	0.21063 (10)	0.0269 (3)	
H14	0.507605	0.282416	0.138239	0.0323*	
C15	0.69513 (13)	0.13760 (11)	0.33140 (11)	0.0319 (4)	
H15	0.720178	0.050302	0.337532	0.0383*	
C16	0.60609 (13)	0.14733 (11)	0.22324 (11)	0.0306 (4)	
H16	0.572119	0.066686	0.158326	0.0367*	
C17	0.74732 (13)	0.25632 (11)	0.43052 (11)	0.0290 (4)	
H17	0.806252	0.249711	0.503227	0.0348*	
C18	0.61995 (12)	0.39388 (10)	0.30999 (10)	0.0227 (3)	
C19	0.75049 (12)	0.52996 (11)	0.50452 (10)	0.0266 (3)	
H19a	0.706391	0.533355	0.589969	0.0319*	
H19b	0.861669	0.557213	0.505998	0.0319*	
C20	0.67537 (13)	0.76766 (11)	0.48737 (10)	0.0293 (4)	
H20a	0.639369	0.784698	0.57656	0.0351*	
H20b	0.601402	0.80254	0.437042	0.0351*	
C21	0.83428 (13)	0.85111 (11)	0.48665 (10)	0.0286 (3)	

H21a	0.83231	0.948073	0.533276	0.0343*	
H21b	0.90867	0.814951	0.535436	0.0343*	
O3	0.51825 (9)	0.58785 (8)	0.24628 (8)	0.0334 (3)	
O4	0.88505 (10)	0.84720 (8)	0.35795 (8)	0.0365 (3)	
H4o	0.9190 (15)	0.7724 (7)	0.3314 (13)	0.0438*	
N2	0.67238 (10)	0.61715 (9)	0.43529 (8)	0.0245 (3)	
O5	0.3877 (11)	0.8415 (9)	0.2889 (9)	0.0357 (3)	0.0838 (15)
C11	0.3327 (18)	0.8496 (16)	0.1646 (10)	0.0268 (4)	0.0838 (15)
H11a	0.40835	0.82158	0.099667	0.0321*	0.0838 (15)
H11b	0.329506	0.947375	0.163376	0.0321*	0.0838 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0204 (5)	0.0222 (5)	0.0221 (5)	0.0032 (4)	−0.0018 (4)	0.0044 (4)
C2	0.0200 (5)	0.0260 (5)	0.0229 (5)	0.0034 (4)	−0.0041 (4)	0.0025 (4)
C3	0.0288 (6)	0.0256 (5)	0.0251 (5)	0.0008 (4)	−0.0027 (4)	0.0070 (4)
C4	0.0306 (6)	0.0221 (5)	0.0405 (6)	0.0070 (5)	−0.0094 (5)	−0.0029 (5)
C5	0.0328 (6)	0.0225 (5)	0.0372 (6)	0.0001 (5)	−0.0099 (5)	0.0077 (5)
C6	0.0246 (6)	0.0293 (6)	0.0285 (5)	0.0062 (4)	−0.0025 (4)	−0.0025 (4)
C7	0.0208 (5)	0.0214 (5)	0.0221 (5)	0.0028 (4)	−0.0038 (4)	0.0032 (4)
C8	0.0227 (5)	0.0287 (5)	0.0225 (5)	0.0043 (4)	0.0019 (4)	0.0054 (4)
C9	0.0265 (6)	0.0227 (5)	0.0343 (6)	0.0059 (4)	−0.0001 (4)	0.0123 (4)
C10	0.0270 (7)	0.0210 (5)	0.0337 (7)	0.0046 (5)	0.0033 (5)	0.0085 (5)
O1	0.0330 (4)	0.0266 (4)	0.0290 (4)	0.0076 (3)	0.0079 (3)	0.0038 (3)
O2	0.0228 (5)	0.0241 (5)	0.0642 (6)	0.0037 (4)	0.0016 (4)	0.0185 (4)
N1	0.0242 (5)	0.0211 (4)	0.0250 (4)	0.0041 (3)	0.0010 (3)	0.0064 (3)
C12	0.0209 (5)	0.0232 (5)	0.0271 (5)	0.0021 (4)	0.0015 (4)	0.0079 (4)
C13	0.0213 (5)	0.0266 (5)	0.0256 (5)	0.0035 (4)	0.0054 (4)	0.0107 (4)
C14	0.0261 (6)	0.0258 (5)	0.0281 (6)	−0.0001 (4)	0.0005 (4)	0.0069 (4)
C15	0.0333 (6)	0.0230 (5)	0.0444 (7)	0.0064 (5)	0.0110 (5)	0.0163 (5)
C16	0.0318 (6)	0.0217 (5)	0.0365 (6)	−0.0010 (4)	0.0076 (5)	0.0055 (4)
C17	0.0276 (6)	0.0325 (6)	0.0327 (6)	0.0066 (5)	0.0046 (5)	0.0177 (5)
C18	0.0213 (5)	0.0216 (5)	0.0265 (5)	0.0019 (4)	0.0037 (4)	0.0088 (4)
C19	0.0256 (6)	0.0304 (6)	0.0246 (5)	0.0047 (4)	0.0009 (4)	0.0079 (4)
C20	0.0293 (6)	0.0237 (5)	0.0326 (6)	0.0059 (4)	0.0051 (5)	0.0006 (4)
C21	0.0318 (6)	0.0234 (5)	0.0290 (6)	0.0037 (4)	0.0030 (4)	0.0028 (4)
O3	0.0361 (5)	0.0276 (4)	0.0383 (5)	0.0077 (3)	−0.0093 (3)	0.0102 (3)
O4	0.0492 (5)	0.0259 (4)	0.0379 (5)	0.0116 (4)	0.0156 (4)	0.0101 (3)
N2	0.0245 (5)	0.0216 (4)	0.0268 (5)	0.0039 (3)	0.0002 (3)	0.0040 (3)
O5	0.0228 (5)	0.0241 (5)	0.0642 (6)	0.0037 (4)	0.0016 (4)	0.0185 (4)
C11	0.0270 (7)	0.0210 (5)	0.0337 (7)	0.0046 (5)	0.0033 (5)	0.0085 (5)

Geometric parameters (Å, °)

C1—C7	1.4760 (14)	C21—O4	1.4121 (14)
C1—O1	1.2419 (12)	O5—C11	1.400 (16)
C1—N1	1.3468 (13)	C3—H3	0.93
C2—C6	1.3888 (14)	C4—H4	0.93

C2—C7	1.3873 (14)	C5—H5	0.93
C2—C8	1.4982 (15)	C6—H6	0.93
C3—C5	1.3842 (15)	C8—H8a	0.97
C3—C7	1.3874 (15)	C8—H8b	0.97
C4—C5	1.3958 (16)	C9—H9a	0.97
C4—C6	1.3895 (17)	C9—H9b	0.97
C8—N1	1.4687 (13)	C10—H10a	0.97
C9—C10	1.5143 (15)	C10—H10b	0.97
C9—N1	1.4552 (13)	O2—H2o	0.820 (12)
C9—C11	1.507 (14)	C14—H14	0.93
C10—O2	1.4146 (15)	C15—H15	0.93
C12—C18	1.4773 (15)	C16—H16	0.93
C12—O3	1.2337 (14)	C17—H17	0.93
C12—N2	1.3544 (12)	C19—H19a	0.97
C13—C17	1.3880 (16)	C19—H19b	0.97
C13—C18	1.3845 (15)	C20—H20a	0.97
C13—C19	1.4995 (13)	C20—H20b	0.97
C14—C16	1.3859 (16)	C21—H21a	0.97
C14—C18	1.3919 (12)	C21—H21b	0.97
C15—C16	1.3898 (17)	O4—H4o	0.820 (9)
C15—C17	1.3930 (14)	O5—H10b	0.909 (9)
C19—N2	1.4651 (15)	C11—H11a	0.97
C20—C21	1.5170 (15)	C11—H11b	0.97
C20—N2	1.4543 (13)		
C7—C1—O1	127.04 (9)	C17—C13—C19	130.72 (10)
C7—C1—N1	106.80 (8)	C18—C13—C19	108.91 (9)
O1—C1—N1	126.15 (9)	C16—C14—C18	117.63 (10)
C6—C2—C7	120.21 (10)	C16—C15—C17	121.09 (11)
C6—C2—C8	130.77 (10)	C14—C16—C15	120.90 (9)
C7—C2—C8	109.02 (9)	C13—C17—C15	118.16 (10)
C5—C3—C7	117.97 (10)	C12—C18—C13	108.93 (8)
C5—C4—C6	121.58 (10)	C12—C18—C14	129.22 (10)
C3—C5—C4	120.26 (11)	C13—C18—C14	121.85 (10)
C2—C6—C4	117.96 (10)	C13—C19—N2	102.64 (8)
C1—C7—C2	108.74 (9)	C21—C20—N2	113.33 (9)
C1—C7—C3	129.27 (9)	C20—C21—O4	112.68 (8)
C2—C7—C3	121.99 (9)	C12—N2—C19	112.86 (8)
C2—C8—N1	102.33 (8)	C12—N2—C20	124.93 (9)
C10—C9—N1	112.90 (10)	C19—N2—C20	122.18 (8)
N1—C9—C11	115.0 (6)	C9—C11—O5	115.3 (10)
C9—C10—O2	112.09 (10)	C10—C11—O2	106.5 (17)
C9—C10—O5	141.7 (5)	H8a—C8—H8b	115.78
O5—C10—C11	108.4 (15)	H9a—C9—H9b	105.81
C1—N1—C8	113.09 (8)	H10a—C10—H10b	106.72
C1—N1—C9	123.93 (8)	H2o—O2—H11a	127.0
C8—N1—C9	122.98 (8)	H19a—C19—H19b	115.53
C18—C12—O3	126.75 (8)	H20a—C20—H20b	105.32
C18—C12—N2	106.64 (9)	H21a—C21—H21b	106.06
O3—C12—N2	126.60 (9)	H11a—C11—H11b	102.9

C17—C13—C18	120.36 (9)

Hydrogen bonds and D—H···π-ring interactions from PLATON (Spek, 2003). Cg1 and Cg2 are the aromatic centroids C2–C7 and C13–C18, respectively (Fig. 1).

D-H···A/*Cg*	D-H	H···A/*Cg*	D···A/*Cg*	D-H···A/*Cg*
O2-H2O···O3	0.820 (11)	1.897 (11)	2.7120 (12)	172.1 (13)
O4-H4O···O1^{i}	0.820 (10)	1.947 (10)	2.7636 (11)	173.6 (12)
C6-H6···O2^{ii}	0.93	2.47	3.2590 (14)	143
C16-H16···O2^{iii}	0.93	2.54	3.2171 (14)	130
C20-H20*b*···O3	0.97	2.57	2.9296 (13)	102
C9-H9a···*Cg*1^{iv}	0.98	2.97	3.4442 (11)	112
C3-H3···*Cg*2^{v}	0.98	2.92	3.6643 (11)	138
C20-H20*a*···*Cg*2^{vi}	0.98	2.84	3.5668 (12)	132

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

Fig. 1

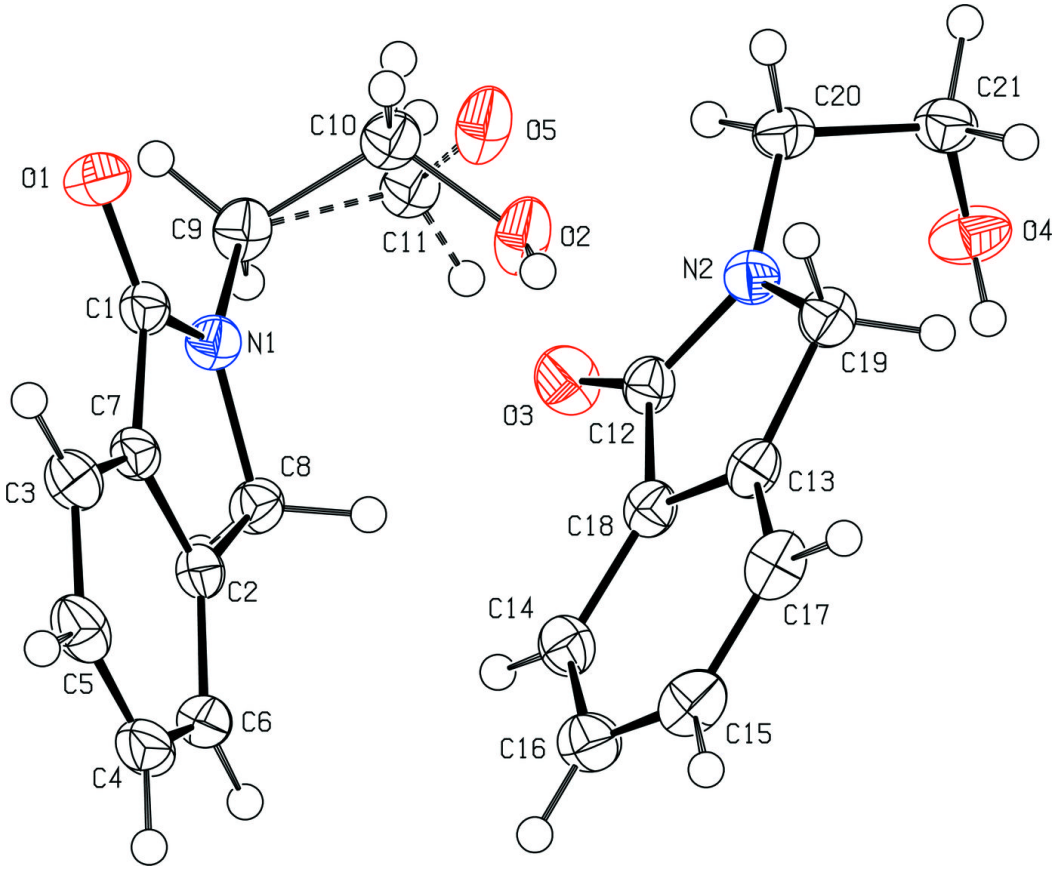
C10
O5
O1
C9
C11
O2
C1
N1
C7
C8
C3
C2
C5
C6
C4
C20
C21
O4
N2
C19
O3
C12
C13
C18
C14
C17
C16
C15

Fig. 2