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Crystal structure of *N*-(3-hydroxyphenyl)succinimide

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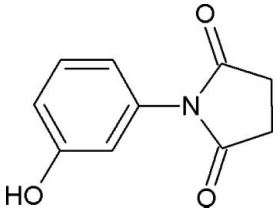
In the title compound, $C_{10}H_9NO_3$, the dihedral angle between the benzene and pyrrolidine rings is 53.9 (1)°. In the crystal, molecules are linked through strong O—H···O hydrogen bonds into zigzag *C*(8) chains running along [010]. The chains are linked by C—H···π interactions forming sheets lying parallel to (100).

Keywords: crystal structure; succinimide; hydrogen bonding.

CCDC reference: 1013858

1. Related literature

For the crystal structures of the 3-methyl and 3-chloro derivatives of *N*-phenylsuccinimide, see: Saraswathi *et al.* (2010, 2011).



2. Experimental

2.1. Crystal data

$C_{10}H_9NO_3$
M_r = 191.18
Monoclinic, $P2_1/c$
a = 11.432 (2) Å
b = 7.6567 (14) Å
c = 10.115 (2) Å
β = 98.688 (7)°
V = 875.2 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.91 mm^{-1}
T = 293 K
0.42 × 0.31 × 0.19 mm

2.2. Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.749, T_{max} = 0.841
3786 measured reflections
1234 independent reflections
1207 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 60.0°

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.140
S = 1.20
1234 reflections
131 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

Cg is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1^{i}	0.94 (4)	1.82 (4)	2.758 (2)	175 (4)
C8—H8*A*···*Cg*^{ii}	0.97	2.83	3.613 (3)	138
C9—H9*A*···*Cg*^{ii}	0.97	2.79	3.579 (3)	139

Symmetry codes: (i) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

Acknowledgements

The authors acknowledge the IOE X-ray diffractometer facility, University of Mysore, India, for the data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: SU2752).

References

Bruker (2009). *APEX2*, *SADABS*, *SAINT-Plus* and *XPREP*. Bruker AXS Inc., Madison, Wisconsin, USA.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Saraswathi, B. S., Foro, S. & Gowda, B. T. (2011). *Acta Cryst.* E**67**, o1977.
Saraswathi, B. S., Gowda, B. T., Foro, S. & Fuess, H. (2010). *Acta Cryst.* E**66**, o1269.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2014). E**70**, o927 [doi:10.1107/S1600536814016328]

Crystal structure of *N*-(3-hydroxyphenyl)succinimide

P. A. Suchetan, S. Naveen, N. K. Lokanath and S. Sreenivasa

S1. Introduction

As a part of a study on the effect of ring and side-chain substitutions on *N*-(Aryl)-succinimides (Saraswathi *et al.*, 2010,2011), the title compound has been synthesized and we report herein on its crystal structure.

S2. Experimental

S2.1. Synthesis and crystallization

The title compound was prepared according to the reported procedure (Saraswathi *et al.*, 2010,2011). Colourless prisms of the title compound were obtained by slow evaporation of an aqueous methanolic solution at room temperature.

S2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydroxyl H atom was located in a difference Fourier map and freely refined. The C-bound H atoms were positioned with idealized geometry and treated as riding atoms: C—H = 0.93-0.97 Å with $U_{iso}(H) = 1.2U_{eq}(C)$.

S3. Results and discussion

The title molecule, Fig. 1, is non-planar with the benzene and pyrrolidine [r.m.s. deviation = 0.039 Å] rings tilted at 53.9 (1) °. This is close to the values of 52.5 (1) and 59.5 (1) ° observed in *N*-(3-methylphenyl)-succinimide (Saraswathi *et al.* 2010) and *N*-(3-chlorophenyl)-succinimide (Saraswathi *et al.* 2011).

In the crystal, molecules are linked through strong O—H···O hydrogen bonds into zigzag C(8) chains running along [010] (Table 1 and Fig. 2). The chains are linked by C—H···π interactions (Table 1 Fig. 3) forming sheets lying parallel to (100).

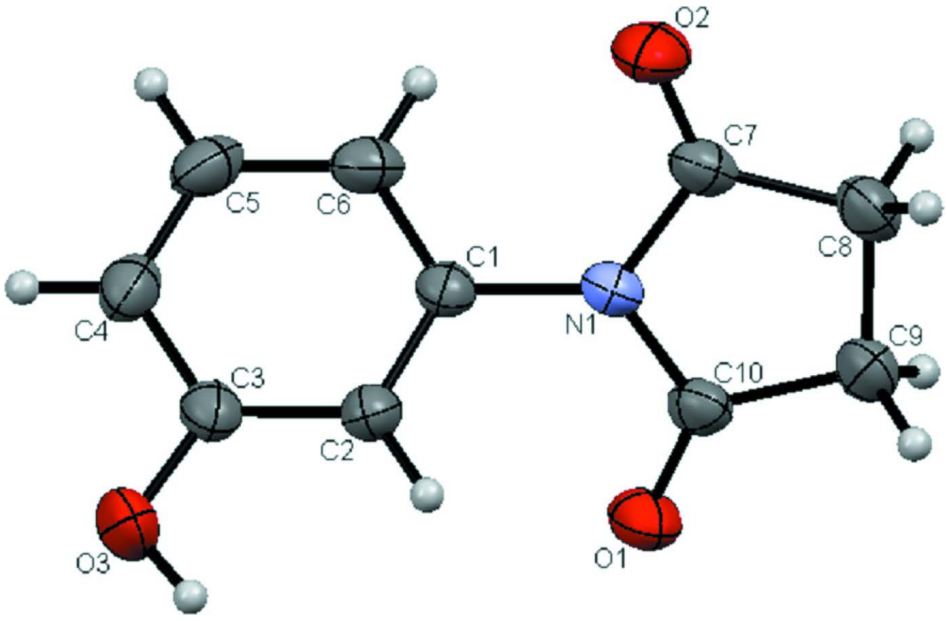


Figure 1

Molecular structure of the title molecule, with atom labeling. Displacement ellipsoids are drawn at the 50% probability level.

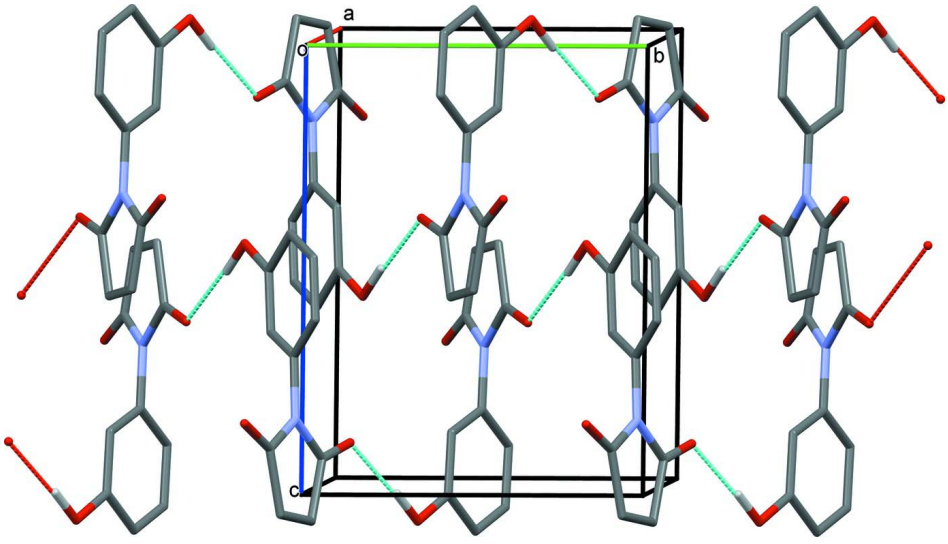


Figure 2

A view along the a axis of the crystal packing of the title compound, showing the formation of the zigzag C(8) chains through O—H···O hydrogen bonds (dashed lines; see Table 1 for details).

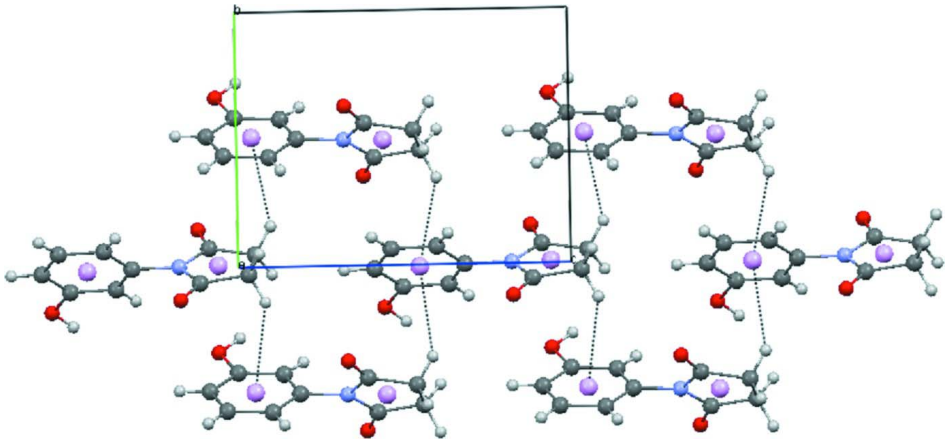


Figure 3

A partial view along the a axis of the crystal packing of the title compound, showing the C—H···π interactions (dashed lines; see Table 1 for details).

1-(3-Hydroxyphenyl)pyrrolidine-2,5-dione

Crystal data

$C_{10}H_9NO_3$
M_r = 191.18
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.432 (2) Å
b = 7.6567 (14) Å
c = 10.115 (2) Å
β = 98.688 (7)°
V = 875.2 (3) Å^3
Z = 4
F(000) = 400

Prism
D_x = 1.451 Mg m^{-3}
Melting point: 393 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 25 reflections
θ = 3.9–60.0°
μ = 0.91 mm^{-1}
T = 293 K
Prism, colourless
0.42 × 0.31 × 0.19 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.749, T_{max} = 0.841

3786 measured reflections
1234 independent reflections
1207 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 60.0°, θ_{min} = 3.9°
$h = -12 \rightarrow 12$
$k = -7 \rightarrow 8$
$l = -5 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.140
S = 1.20
1234 reflections
131 parameters
0 restraints

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

$w = 1/[\sigma^2(F_o^2) + (0.0766P)^2 + 0.2946P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.91904 (12)	0.1492 (2)	0.88087 (15)	0.0436 (5)
O2	0.56202 (12)	−0.1251 (2)	0.82562 (16)	0.0482 (5)
O3	0.92280 (13)	−0.1661 (2)	0.43867 (15)	0.0454 (5)
N1	0.74293 (13)	0.0058 (2)	0.82293 (16)	0.0293 (5)
C1	0.74308 (15)	−0.0001 (2)	0.68070 (19)	0.0281 (6)
C2	0.83725 (16)	−0.0782 (2)	0.63281 (18)	0.0300 (6)
C3	0.83605 (17)	−0.0861 (3)	0.49542 (19)	0.0326 (6)
C4	0.74209 (18)	−0.0147 (3)	0.4099 (2)	0.0391 (7)
C5	0.64917 (18)	0.0627 (3)	0.4603 (2)	0.0407 (7)
C6	0.64839 (17)	0.0704 (3)	0.5970 (2)	0.0361 (6)
C7	0.65000 (16)	−0.0592 (2)	0.8850 (2)	0.0327 (6)
C8	0.68144 (17)	−0.0292 (3)	1.0320 (2)	0.0374 (7)
C9	0.80476 (18)	0.0493 (3)	1.0518 (2)	0.0367 (6)
C10	0.83298 (16)	0.0764 (2)	0.91334 (19)	0.0313 (6)
H2	0.90020	−0.12450	0.69140	0.0360*
H3	0.978 (3)	−0.223 (5)	0.502 (4)	0.088 (10)*
H4	0.74170	−0.01900	0.31800	0.0470*
H5	0.58650	0.11000	0.40200	0.0490*
H6	0.58570	0.12170	0.63140	0.0430*
H8A	0.68090	−0.13840	1.08050	0.0450*
H8B	0.62560	0.05040	1.06340	0.0450*
H9A	0.80610	0.15940	1.09940	0.0440*
H9B	0.86130	−0.02960	1.10190	0.0440*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0306 (8)	0.0573 (10)	0.0443 (9)	−0.0123 (7)	0.0103 (7)	−0.0083 (7)
O2	0.0306 (8)	0.0641 (10)	0.0501 (9)	−0.0141 (7)	0.0066 (7)	0.0068 (8)
O3	0.0417 (9)	0.0634 (10)	0.0328 (9)	0.0051 (7)	0.0110 (7)	−0.0054 (7)
N1	0.0224 (8)	0.0360 (9)	0.0305 (9)	−0.0012 (6)	0.0071 (6)	0.0000 (6)
C1	0.0248 (10)	0.0305 (10)	0.0290 (10)	−0.0052 (7)	0.0045 (8)	0.0009 (7)
C2	0.0248 (10)	0.0362 (11)	0.0283 (10)	−0.0014 (8)	0.0021 (8)	0.0010 (8)

C3	0.0302 (10)	0.0375 (11)	0.0304 (10)	−0.0074 (8)	0.0060 (8)	−0.0009 (8)
C4	0.0377 (12)	0.0478 (13)	0.0299 (10)	−0.0099 (9)	−0.0010 (9)	0.0044 (9)
C5	0.0308 (11)	0.0470 (13)	0.0406 (12)	−0.0039 (9)	−0.0067 (9)	0.0116 (9)
C6	0.0241 (10)	0.0386 (11)	0.0452 (12)	−0.0010 (8)	0.0043 (8)	0.0051 (9)
C7	0.0250 (10)	0.0340 (10)	0.0405 (11)	0.0024 (8)	0.0100 (9)	0.0054 (8)
C8	0.0349 (11)	0.0431 (12)	0.0371 (11)	0.0054 (8)	0.0151 (9)	0.0020 (8)
C9	0.0333 (11)	0.0447 (11)	0.0333 (11)	0.0060 (9)	0.0085 (8)	−0.0043 (9)
C10	0.0250 (10)	0.0345 (11)	0.0353 (11)	0.0028 (8)	0.0072 (8)	−0.0048 (8)

Geometric parameters (Å, º)

O1—C10	1.218 (2)	C5—C6	1.385 (3)
O2—C7	1.202 (2)	C7—C8	1.494 (3)
O3—C3	1.364 (3)	C8—C9	1.518 (3)
O3—H3	0.94 (4)	C9—C10	1.498 (3)
N1—C1	1.440 (2)	C2—H2	0.9300
N1—C7	1.404 (2)	C4—H4	0.9300
N1—C10	1.380 (2)	C5—H5	0.9300
C1—C2	1.382 (2)	C6—H6	0.9300
C1—C6	1.380 (3)	C8—H8A	0.9700
C2—C3	1.389 (3)	C8—H8B	0.9700
C3—C4	1.386 (3)	C9—H9A	0.9700
C4—C5	1.380 (3)	C9—H9B	0.9700
C3—O3—H3	112 (2)	N1—C10—C9	108.71 (16)
C1—N1—C10	124.14 (15)	O1—C10—N1	123.55 (18)
C7—N1—C10	112.43 (16)	C1—C2—H2	121.00
C1—N1—C7	123.43 (15)	C3—C2—H2	121.00
N1—C1—C6	118.80 (16)	C3—C4—H4	120.00
C2—C1—C6	122.34 (18)	C5—C4—H4	120.00
N1—C1—C2	118.85 (16)	C4—C5—H5	120.00
C1—C2—C3	118.63 (17)	C6—C5—H5	120.00
O3—C3—C4	117.31 (17)	C1—C6—H6	121.00
C2—C3—C4	119.80 (18)	C5—C6—H6	121.00
O3—C3—C2	122.87 (18)	C7—C8—H8A	111.00
C3—C4—C5	120.42 (19)	C7—C8—H8B	111.00
C4—C5—C6	120.57 (19)	C9—C8—H8A	111.00
C1—C6—C5	118.24 (19)	C9—C8—H8B	111.00
O2—C7—N1	123.91 (18)	H8A—C8—H8B	109.00
N1—C7—C8	107.82 (16)	C8—C9—H9A	111.00
O2—C7—C8	128.27 (18)	C8—C9—H9B	111.00
C7—C8—C9	105.74 (16)	C10—C9—H9A	111.00
C8—C9—C10	104.97 (16)	C10—C9—H9B	111.00
O1—C10—C9	127.74 (18)	H9A—C9—H9B	109.00
C7—N1—C1—C2	−125.04 (18)	N1—C1—C2—C3	178.96 (16)
C10—N1—C1—C2	55.4 (2)	C2—C1—C6—C5	−0.4 (3)
C7—N1—C1—C6	54.1 (2)	C1—C2—C3—C4	0.7 (3)

C10—N1—C1—C6	−125.46 (19)	C1—C2—C3—O3	−177.55 (17)
C7—N1—C10—C9	3.7 (2)	C2—C3—C4—C5	−0.6 (3)
C1—N1—C10—O1	4.0 (3)	O3—C3—C4—C5	177.7 (2)
C7—N1—C10—O1	−175.62 (16)	C3—C4—C5—C6	0.1 (3)
C1—N1—C7—O2	−0.3 (3)	C4—C5—C6—C1	0.4 (3)
C10—N1—C7—C8	−0.1 (2)	O2—C7—C8—C9	177.14 (19)
C10—N1—C7—O2	179.37 (17)	N1—C7—C8—C9	−3.4 (2)
C1—N1—C10—C9	−176.69 (16)	C7—C8—C9—C10	5.3 (2)
C1—N1—C7—C8	−179.75 (16)	C8—C9—C10—O1	173.70 (18)
C6—C1—C2—C3	−0.2 (3)	C8—C9—C10—N1	−5.6 (2)
N1—C1—C6—C5	−179.51 (18)		

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1^{i}	0.94 (4)	1.82 (4)	2.758 (2)	175 (4)
C8—H8*A*···*Cg*^{ii}	0.97	2.83	3.613 (3)	138
C9—H9*A*···*Cg*^{ii}	0.97	2.79	3.579 (3)	139

Symmetry codes: (i) −*x*+2, *y*−1/2, −*z*+3/2; (ii) *x*, −*y*+3/2, *z*+1/2.