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N-Hydroxysuccinimide

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Key indicators

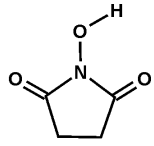
Single-crystal X-ray study
T = 133 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.108
Data-to-parameter ratio = 11.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The molecule of the title compound, $C_4H_5NO_3$, is planar (mean deviation of non-H atoms 0.03 Å). The N—C bond lengths are significantly different [1.365 (2) and 1.392 (2) Å]. The C═O group associated with the shorter N—C bond accepts a classical intermolecular hydrogen bond from the hydroxy H atom.

Comment

N-Hydroxysuccinimide, (I), has found applications in the analysis of amines, with which it readily forms crystalline adducts. The structure of one of these, with *p*-chlorobenzylamine, was determined (Reck & Adam, 1977), and it was established that the amine is in the protonated form, while the hydroxy group is deprotonated. However, the structure of *N*-hydroxysuccinimide itself has not previously been determined; it is presented here.



(I)

The molecule is shown in Fig. 1; it is planar within a mean deviation (non-H atoms) of 0.03 Å. The most striking feature of the molecular dimensions is the large difference between the chemically equivalent bond lengths N—C1 [1.365 (2) Å] and N—C4 [1.392 (2) Å]. If this is accepted as genuine, one possible explanation would be delocalization of the lone pair at nitrogen preferentially in the direction of O1 [*cf.* the corresponding C═O bond lengths of 1.224 (2) and 1.207 (2) Å]. This would be consistent with the fact that atom O1 accepts a classical intermolecular hydrogen bond from the OH group. The structures of the above-mentioned adduct and of *N*-hydroxyphthalimide (Miao *et al.*, 1995) are available for comparison; in the former, the corresponding N—C bond

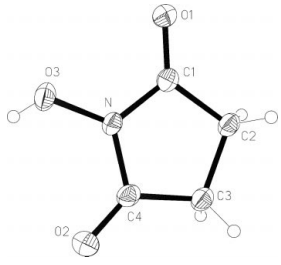


Figure 1
The molecule of the title compound in the crystal. Ellipsoids are drawn at the 50% probability level. H-atom radii are arbitrary.

lengths are 1.365 and 1.376 Å, and in the latter 1.384 (6) and 1.397 (8) Å. In each case, the first bond length involves the C═O group that accepts a classical hydrogen bond, whereas the latter C═O group does not. The differences are, however, not significant.

The classical hydrogen bond and one short C—H···O interaction connect the molecules to form ribbons parallel to the *a* axis (Fig. 2).

Experimental

A commercial sample of the title compound (Aldrich) proved to contain single crystals.

Crystal data

$C_4H_5NO_3$
M_r = 115.09
Orthorhombic, $P2_12_12_1$
a = 5.4266 (8) Å
b = 7.2419 (12) Å
c = 12.445 (2) Å
V = 489.09 (13) Å^3
Z = 4
D_x = 1.563 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3627 reflections
θ = 2.8–30.5°
μ = 0.14 mm^{-1}
T = 133 (2) K
Irregular tablet, colourless
0.30 × 0.25 × 0.10 mm

Data collection

Bruker SMART 1000 CCD diffractometer
ω scans
Absorption correction: none
5566 measured reflections
860 independent reflections
803 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 30.0°
$h = -7 \rightarrow 7$
$k = -10 \rightarrow 10$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.109
S = 1.05
860 reflections
77 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0857P)^2 + 0.0226P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.224 (2)	C3—C4	1.502 (2)
C1—N	1.365 (2)	C4—O2	1.207 (2)
C1—C2	1.507 (2)	C4—N	1.392 (2)
C2—C3	1.539 (2)	N—O3	1.3769 (16)
O1—C1—N	124.65 (13)	O2—C4—C3	129.80 (14)
O1—C1—C2	127.90 (13)	N—C4—C3	106.65 (13)
N—C1—C2	107.44 (12)	C1—N—O3	121.03 (12)
C1—C2—C3	105.01 (13)	C1—N—C4	115.22 (12)
C4—C3—C2	105.20 (12)	O3—N—C4	123.17 (12)
O2—C4—N	123.54 (14)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H0···O1^{i}	0.97 (3)	1.71 (3)	2.6442 (16)	161 (3)
C3—H3A···O1^{ii}	0.99	2.49	3.320 (2)	142
C2—H2B···O2^{iii}	0.99	2.60	3.585 (2)	174

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

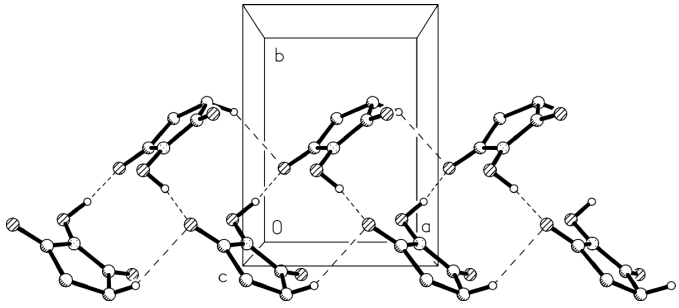


Figure 2
Packing diagram of the title compound, viewed parallel to the *c* axis. Hydrogen bonds are indicated by dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity.

The hydroxy H atom was refined freely. Other H atoms were included using a riding model with fixed C—H bond lengths of 0.99 Å; U_{iso}(H) values were fixed at 1.2 times U_{eq} of the parent atom. The absolute structure could not be determined because the anomalous scattering effects were too small, and Friedel opposite reflections were therefore merged. The Flack (1983) parameter is meaningless in such cases. The compound is not chiral, and the concept of absolute configuration does not apply. A rigid-body libration correction (Schomaker & Trueblood, 1968) led to the following corrected bond lengths (Å): C1—C2 1.510, C2—C3 1.544, C3—C4 1.506, C1—N 1.369, C4—N 1.395, C1—O1 1.227, C4—O2 1.210 and N—O3 1.380.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

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