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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates for (I) and (II), angles for (I) and bond lengths and angles for (II), have been deposited with the IUCr (Reference: AS1120). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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N-Hydroxyphthalimide

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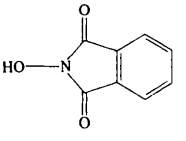
Abstract

The title compound, *N*-hydroxy-1*H*-isoindole-1,3(2*H*)-dione, $C_8H_5NO_3$, is virtually planar with a maximum deviation of 0.03 (1) Å from planarity. Molecules are connected *via* hydrogen bonds and van der Waals interactions.

Comment

The title molecule, (I), is planar with a maximum deviation from the molecular plane of 0.03 (1) Å and a dihedral angle between the five- and six-membered ring planes of 0.66 (7)°. These features are similar to those found in ninhydrin (Medrud, 1969). Our interest is in comparing the geometries of the hydroxamic and amidic groups. Compared with the structure of phthalic anhydride (Bates & Cutler, 1977), the structure of the title compound shows only small differences in bond lengths between chemically equivalent atoms, but the N(1)—C(1)—O(1) [124.6 (5)°] and N(1)—C(2)—O(2) [124.9 (5)°] bond angles are about 4° larger than the corresponding angles of phthalic anhydride (120.5 and 120.6°, respectively) and are close to the corresponding angles in *N*-phthaloylglycine hydroxamic acid form (I) (123.5 and 124.0°, respectively) and form (II) (123.5 and 124.3°, respectively) (Sikirica & Vickovic, 1980, 1981).



(I)

The crystal structure is characterized by intermolecular hydrogen bonds: O(10)···O(1^{i}) 2.69 (1) Å and O(10)—H(10)···O(1^{i}) 167 (3)° [symmetry code: (i) $2-x$, $\frac{1}{2}+y$, $\frac{1}{2}-z$]. These values are in good agreement with the values for salicylhydroxamic acid (Larsen, 1978), acetohydroxamic acid hemihydrate (Bracher & Small, 1970) and *N*-(3-cyanophenyl)acetohydroxamic acid hydrate (Mocharla, Powell & van der Helm, 1984).

The molecular packing is stabilized by hydrogen bonds and van der Waals interactions. In the **b** direction, the molecules are linked into chains by hydrogen bonds.

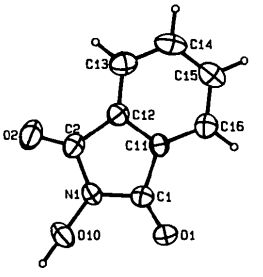


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are plotted at the 50% probability level.

Experimental

Crystal data

$C_8H_5NO_3$
M_r = 163.13

Mo $K\alpha$ radiation
λ = 0.71073 Å

Monoclinic
$P2_1/c$
a = 11.549 (3) Å
b = 3.756 (1) Å
c = 16.442 (8) Å
β = 104.94 (3)°
V = 689.1 (4) Å^3
Z = 4
D_x = 1.572 Mg m^{-3}
D_m = 1.58 Mg m^{-3}

Cell parameters from 25 reflections
θ = 5.42–9.50°
μ = 0.1151 mm^{-1}
T = 298 K
Prism
0.5 × 0.4 × 0.25 mm
Colourless
Crystal source: from water solution

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical
T_{min} = 0.8358, T_{max} = 0.9992
1309 measured reflections
1262 independent reflections

536 observed reflections [$F_o > 3\sigma(F_o)$]
R_{int} = 0.032
θ_{max} = 24°
$h = -13 \rightarrow 13$
$k = 0 \rightarrow 4$
$l = 0 \rightarrow 18$
3 standard reflections
frequency: 150 min
intensity decay: 0.5%

Refinement

Refinement on F
R = 0.041
wR = 0.045
S = 0.685
535 reflections
125 parameters
Only coordinates of H atoms refined

If $F < 61$ then $w = 1$, if $F \geq 61$ then $w = (61/F)^2$, if $F^2 < 3\sigma(F^2)$ then $w = 0$
$(\Delta/\sigma)_{max}$ = 0.01
$\Delta\rho_{max}$ = 0.169 e Å^{-3}
$\Delta\rho_{min}$ = −0.189 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
O(10)	0.8854 (3)	0.195 (1)	0.2014 (2)	3.83 (8)
O(1)	0.9829 (3)	0.102 (1)	0.3745 (1)	3.49 (8)
O(2)	0.6619 (3)	0.557 (1)	0.1790 (2)	4.66 (9)
N(1)	0.8393 (3)	0.336 (1)	0.2635 (3)	3.02 (9)
C(1)	0.8895 (4)	0.262 (1)	0.3477 (3)	2.7 (1)
C(2)	0.7250 (4)	0.486 (1)	0.2480 (3)	2.8 (1)
C(11)	0.8037 (4)	0.403 (1)	0.3915 (3)	2.5 (1)
C(12)	0.7038 (4)	0.535 (1)	0.3317 (3)	2.7 (1)
C(13)	0.6074 (4)	0.673 (2)	0.3556 (3)	3.5 (1)
C(14)	0.6132 (4)	0.677 (2)	0.4403 (3)	4.1 (1)
C(15)	0.7122 (5)	0.549 (2)	0.5002 (3)	4.0 (1)
C(16)	0.8084 (4)	0.409 (1)	0.4758 (3)	3.4 (1)

Table 2. *Selected geometric parameters* (Å, °)

O(10)—N(1)	1.374 (5)	C(11)—C(12)	1.399 (6)
O(1)—C(1)	1.213 (5)	C(11)—C(16)	1.372 (7)
O(2)—C(2)	1.209 (5)	C(12)—C(13)	1.374 (7)
N(1)—C(1)	1.384 (6)	C(13)—C(14)	1.377 (8)
N(1)—C(2)	1.397 (8)	C(14)—C(15)	1.388 (8)
C(1)—C(11)	1.467 (6)	C(15)—C(16)	1.379 (8)
C(2)—C(12)	1.470 (7)		
O(10)—N(1)—C(1)	121.5 (4)	C(1)—C(11)—C(12)	108.8 (4)
O(10)—N(1)—C(2)	123.3 (4)	C(1)—C(11)—C(16)	130.2 (5)
C(1)—N(1)—C(2)	113.4 (4)	C(12)—C(11)—C(16)	121.0 (5)
O(1)—C(1)—N(1)	124.6 (5)	C(2)—C(12)—C(11)	108.0 (4)
O(1)—C(1)—C(11)	130.6 (4)	C(2)—C(12)—C(13)	131.0 (5)
N(1)—C(1)—C(11)	104.8 (4)	C(11)—C(12)—C(13)	121.0 (5)
O(2)—C(2)—N(1)	124.9 (4)	C(12)—C(13)—C(14)	117.5 (5)
O(2)—C(2)—C(12)	130.2 (5)	C(13)—C(14)—C(15)	122.0 (6)
N(1)—C(2)—C(12)	104.8 (4)	C(14)—C(15)—C(16)	120.2 (5)
C(11)—C(16)—C(15)	118.3 (5)		

Program used throughout the analysis: *MolEN* (Fair, 1990). Program used to solve the structure: *MULTAN*11/82 (Main *et al.*, 1982).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry, including H-atom geometry and torsion angles, have been deposited with the IUCr (Reference: AS1104). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A Branched Polysilane

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Abstract

2,2,5,5-Tetrakis(trimethylsilyl)-1,1,1,3,3,4,4,6,6,6-decamethylhexasilane, $C_{22}H_{66}Si_{10}$, is a polysilane in which the longest chain is made up of six Si atoms and branching occurs at the second and fifth Si atoms. Each of the two central Si atoms is bonded to a tris(trimethylsilyl)silyl group in an *anti* arrangement. Bond lengths and angles are sufficiently close to normal to indicate that the molecule is relatively unstrained.