N(2)—C(3)	1.399 (4)	C(5)—C(51)	1.493 (4)
C(3)—O(3)	1.194 (3)	C(5)—C(52)	1.468 (4)
C(3)—N(4)	1.316 (4)		
O(1)—N(1)—N(2)	125.1 (2)	C(3)—N(4)—C(5)	112.5 (2)
O(1)—N(1)—C(5)	120.4 (2)	N(4)—C(5)—N(1)	97.7 (2)
N(2)—N(1)—C(5)	114.5 (2)	N(1)—C(5)—C(51)	109.5 (2)
N(1)—N(2)—C(3)	105.5 (2)	N(1)—C(5)—C(52)	106.8 (2)
N(2)—C(3)—O(3)	121.4 (3)	N(4)—C(5)—C(51)	113.4 (2)
N(2)—C(3)—N(4)	109.7 (2)	N(4)—C(5)—C(52)	113.0 (2)
O(3)—C(3)—N(4)	128.9 (3)	C(51)—C(5)—C(52)	114.8 (3)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N(4)—H···O(3^{i})	1.44 (4)	1.41 (4)	2.841 (3)	170 (3)

Symmetry code: (i) $1-x, 1-y, -z$.

The structure was solved using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). All remaining calculations were performed with a local version of the *NRC* program system (Ahmed & Singh, 1973).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and least-squares-planes data have been deposited with the IUCr (Reference: HA1112). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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N-(Propargyloxy)phthalimide

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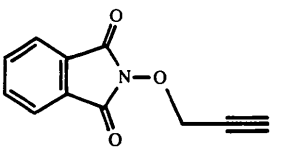
Abstract

The structure of the title compound, *N*-(2-propynyloxy)-phthalimide, $C_{11}H_7NO_3$, consists of C≡C—H···O=C hydrogen-bonded dimers having C···O separations of 3.28 Å.

Comment

The molecular structure of *N*-(propargyloxy)phthalimide, (I), allows the prediction of interesting C—H···O hydrogen-bonding properties, because it contains three O atoms as hydrogen-bond acceptors and only C—H hydrogen-bond donors. In fact, the molecule forms three short C—H···O contacts (Table 3) so that each of its O atoms can accept at least one, admittedly weak, hydrogen bond.



(I)

Pairs of molecules, related by the space group inversion center, are connected by mutual C≡C—H···O=C interactions (Fig. 1), with C···O and H_{norm}···O separations of 3.28 (8) and 2.27 Å, respectively (Table 3), for a normalized H-atom position. To verify the bonding nature of this contact, the alkynyl C—H stretching frequency was determined by IR spectroscopy for molecules in apolar solvent and also for molecules in the crystalline state: ν_{CH} = 3312 cm^{-1} (CCl_4) and 3253 cm^{-1} (KBr). The downshift of 59 cm^{-1} due to hydrogen bonding is in the expected range for this type of C···O separation (Desiraju, 1991, and references therein).

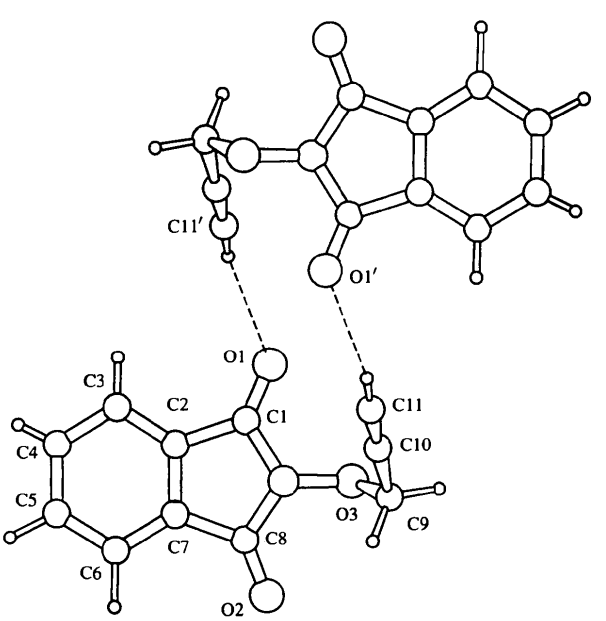


Fig. 1. The molecular structure, labelling scheme and mutual C≡C—H···O=C hydrogen bonding of a pair of symmetry-related molecules (*ORTEP*II; Johnson, 1976).

Experimental

The title compound was commercially available (Aldrich) and was recrystallized from methanol.

Crystal data

$C_{11}H_7NO_3$
$M_r = 201.8$
Monoclinic
$P2_1/a$
$a = 7.838\ (4)$ Å
$b = 15.318\ (4)$ Å
$c = 8.840\ (4)$ Å
$\beta = 116.22\ (4)°$
$V = 952.1\ (8)$ Å^3
$Z = 4$
$D_x = 1.40$ Mg m^{-3}
Cu $K\alpha$ radiation
$\lambda = 1.54184$ Å
Cell parameters from 25 reflections
$\theta = 10.8–33.6°$
$\mu = 0.83$ mm^{-1}
$T = 295$ K
Plate
0.5 × 0.4 × 0.04 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: refined from ΔF (*DIFABS*; Walker & Stuart, 1983)
$T_{min} = 0.66$, $T_{max} = 0.97$
1584 measured reflections
1368 independent reflections
1008 observed reflections $[F > 3\sigma(F)]$
$R_{int} = 0.056$
$\theta_{max} = 60°$
$h = -8 \rightarrow 8$
$k = 0 \rightarrow 17$
$l = 0 \rightarrow 9$
3 standard reflections
frequency: 60 min
intensity decay: 1.4%

Refinement

Refinement on F
$R = 0.049$
$wR = 0.049$
$S = 1.00$
1008 reflections
164 parameters
H atoms refined isotropically
Unit weights applied
$(\Delta/\sigma)_{max} = 0.013$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Atomic scattering factors from *SHELX*76 (Sheldrick, 1976)

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

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
N	0.1455 (5)	0.1898 (2)	0.3249 (5)	0.040 (4)
O1	0.2674 (5)	0.0699 (2)	0.2475 (4)	0.056 (4)
O2	0.0816 (5)	0.2931 (2)	0.4840 (4)	0.049 (4)
O3	0.1637 (4)	0.2473 (2)	0.2122 (4)	0.047 (3)
C1	0.2202 (6)	0.1055 (3)	0.3444 (6)	0.039 (5)
C2	0.2224 (6)	0.0749 (3)	0.5053 (6)	0.036 (4)
C3	0.2693 (7)	−0.0054 (3)	0.5817 (7)	0.047 (5)
C4	0.2518 (8)	−0.0152 (4)	0.7314 (8)	0.056 (6)
C5	0.1899 (8)	0.0505 (4)	0.7986 (7)	0.055 (6)
C6	0.1411 (7)	0.1311 (3)	0.7207 (6)	0.046 (5)
C7	0.1610 (6)	0.1419 (3)	0.5734 (6)	0.036 (4)
C8	0.1224 (6)	0.2200 (3)	0.4645 (6)	0.036 (5)
C9	−0.0246 (7)	0.2673 (3)	0.0738 (6)	0.045 (5)
C10	−0.1197 (7)	0.1907 (4)	−0.0201 (6)	0.048 (5)
C11	−0.2025 (10)	0.1305 (4)	−0.1008 (8)	0.066 (7)

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

N—C1	1.397 (6)	O2—C8	1.198 (6)
N—C8	1.403 (7)	O3—C9	1.475 (5)
N—O3	1.383 (6)	C9—C10	1.440 (7)
O1—C1	1.204 (7)	C10—C11	1.171 (8)
C1—N—C8	114.0 (4)	C9—O3—N	110.2 (4)
C1—N—O3	120.4 (4)	C10—C9—O3	112.5 (4)
C8—N—O3	121.2 (4)	C9—C10—C11	177.3 (6)
O3—N—C8—O2	14.5 (7)	C8—N—O3—C9	−90.8 (5)
O3—N—C1—O1	−16.3 (8)	N—O3—C9—C10	−60.5 (5)
C1—N—O3—C9	114.1 (5)		

Table 3. *Hydrogen-bonding geometry* (Å, °)

	C—H	H···O	C···O	H_{norm}···O	C—H_{norm}···O
C3—H3···O2^i	1.00 (5)	2.52 (5)	3.439 (7)	2.43	153
C9—H92···O3^{ii}	1.07 (5)	2.23 (5)	3.187 (8)	2.21	149
C11—H11···O1^{iii}	0.83 (6)	2.50 (7)	3.283 (8)	2.27	154

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

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *CAD*-4 *Software*. Structure solution: *SHELXS*86 (Sheldrick, 1985). Structure refinement: *SHELX*76 (Sheldrick, 1976). Molecular graphics: *ORTEP*II (Johnson, 1976).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: SE1071). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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