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3-(2-Biphenyl)sydnone

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Key indicators

Single-crystal synchrotron study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.146
Data-to-parameter ratio = 13.6

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

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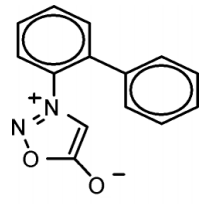
The title compound, $C_{14}H_{10}N_2O_2$, is one of many sydnones which have been synthesized in order to investigate the influence of substituents and sydnone-ring stability. There is medicinal interest in the sydnone if the ring can predictably release NO. Bond lengths and angles of the sydnone ring were compared with those of other published sydnone compounds and were found to fit the average of the published data.

Comment

The title compound, (I), is part of a series of sydnones which have been produced in order to detect the influence of substituents on the sydnone ring. The aim is to find substituents which will influence the ring in a way that will cause the breaking of the N2—N3 and O1—C5 bonds.



(I)

The molecular structure of (I) is shown in Fig. 1, and selected bond distances and angles are given in Table 1. The observed structural data were compared with the data for other, previously published, sydnones found in the Cambridge Structural Database (CSD, Version 5.22; Allen, 2002). While most bonds of the sydnone ring are close to average values, the C4—C5 bond is observed to be 1.382 (3) Å, which is slightly smaller than the average of 1.406 (4) Å from the CSD data. Bond angles do not exhibit a significant deviation from average values.

The planes of the sydnone ring and the attached phenyl ring are twisted by 58.97 (12)° from each other. The plane of the second phenyl ring in the 2′ position is twisted by 50.16 (11)° from the phenyl ring attached to the sydnone, making the molecule markedly non-planar. In the crystal structure of (I), there are two significant C—H···O intermolecular contacts linking symmetry-related molecules, as shown in Table 2.

Experimental

Compound (I) was prepared by reacting 3-(2-bromophenyl)sydnone with phenylboric acid, and was then recrystallized from dichloromethane and hexane (Weisner, 2003).

Crystal data

$C_{14}H_{10}N_2O_2$
$M_r = 238.24$
Monoclinic, $P2_1/n$
$a = 11.012\ (15)$ Å
$b = 8.310\ (15)$ Å
$c = 12.941\ (15)$ Å
$\beta = 108.406\ (15)^\circ$
$V = 1124\ (3)$ Å^3
$Z = 4$
$D_x = 1.408$ Mg m^{-3}
Synchrotron radiation, $\lambda = 0.70998$ Å
Cell parameters from 25 reflections
$\theta = 12$–18°
$\mu = 0.10$ mm^{-1}
$T = 298\ (2)$ K
Block, colorless
0.40 × 0.35 × 0.10 mm

Data collection

Mar CCD area-detector diffractometer
ω scans
Absorption correction: none
16 475 measured reflections
2210 independent reflections
2019 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 26.7^\circ$
$h = -13 \rightarrow 13$
$k = -10 \rightarrow 10$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.146$
$S = 1.13$
2210 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0767P)^2 + 0.6398P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O5—C5	1.211 (2)	C2′—C7	1.486 (3)
O1—N2	1.378 (3)	N3—C4	1.335 (2)
O1—C5	1.415 (2)	C3′—C4′	1.386 (3)
N2—N3	1.311 (2)	C4—C5	1.407 (3)
C1′—C6′	1.384 (3)	C7—C8	1.393 (3)
C1′—C2′	1.393 (3)	C7—C12	1.400 (3)
C1′—N3	1.442 (3)	C8—C9	1.384 (3)
C5′—C4′	1.382 (3)	C9—C10	1.388 (3)
C5′—C6′	1.385 (3)	C10—C11	1.387 (3)
C2′—C3′	1.397 (3)	C11—C12	1.387 (3)
N2—O1—C5	111.06 (12)	C5′—C4′—C3′	120.91 (17)
N3—N2—O1	103.66 (14)	N3—C4—C5	106.47 (15)
C6′—C1′—C2′	123.41 (17)	O5—C5—C4	136.77 (16)
C6′—C1′—N3	115.84 (17)	O5—C5—O1	119.87 (15)
C2′—C1′—N3	120.74 (14)	C4—C5—O1	103.35 (14)
C4′—C5′—C6′	119.33 (15)	C8—C7—C12	118.88 (15)
C1′—C2′—C3′	116.14 (15)	C8—C7—C2′	120.51 (16)
C1′—C2′—C7	123.25 (16)	C12—C7—C2′	120.58 (16)
C3′—C2′—C7	120.56 (18)	C9—C8—C7	120.43 (17)
N2—N3—C4	115.44 (15)	C8—C9—C10	120.38 (17)
N2—N3—C1′	116.74 (13)	C11—C10—C9	119.81 (16)
C4—N3—C1′	127.66 (13)	C10—C11—C12	119.98 (17)
C1′—C6′—C5′	118.91 (18)	C11—C12—C7	120.52 (17)
C4′—C3′—C2′	121.27 (19)		

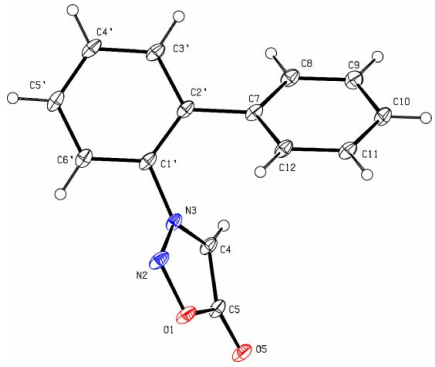


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and with displacement ellipsoids at the 30% probability level. H atoms are shown as small spheres of arbitrary radii.

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O5^{i}	0.93	2.36	3.214 (6)	152
C6′—H6′···O1^{ii}	0.93	2.60	3.335 (6)	136

Symmetry codes: (i) $1-x, 2-y, 2-z$; (ii) $\frac{1}{2}-x, y-\frac{1}{2}, \frac{5}{2}-z$.

H atoms were included in calculated positions and treated as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.5U_{eq}(C)$.

Data collection: *MarControl* (MARResearch, 2000); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Fox & Holmes, 1966); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1994); software used to prepare material for publication: *OSCAIL* (McArdle, 2003).

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References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Fox, G. & Holmes, K. (1966). *Acta Cryst.* **20**, 886–881.
MARResearch (2000). *MARControl*. MARResearch, Germany.
McArdle, P. (1994). *J. Appl. Cryst.* **27**, 438–439.
McArdle, P. (2003). *OSCAIL for Windows*. Version 10. Crystallography Centre, Chemistry Department, NUI Galway, Ireland.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Weisner, A. (2003). MSc. thesis, Wright State University, USA.