C37—N1—C7	118.3 (3)	C80—N3—C50	116.5 (3)
C1—N1—C7	117.9 (3)	C44—N3—C50	118.9 (3)
C10—N2—C9	117.1 (3)	C53—N4—C49	120.6 (3)
C10—N2—C6	117.9 (3)	C53—N4—C52	116.3 (3)
C9—N2—C6	123.3 (3)	C49—N4—C52	122.6 (3)
C6—C1—N1	118.9 (3)	C49—C44—N3	120.9 (3)
C2—C1—N1	121.5 (3)	C45—C44—N3	120.0 (3)
C1—C6—N2	120.6 (3)	C44—C49—N4	121.1 (3)
N1—C7—C31	111.8 (3)	N3—C50—C74	112.5 (3)
N1—C7—C8	110.4 (3)	N3—C50—C51	110.1 (3)
C31—C7—C8	112.3 (3)	C74—C50—C51	112.1 (3)
C9—C8—C7	114.4 (3)	C52—C51—C50	113.6 (3)
N2—C9—C8	112.5 (3)	O6—C52—C51	103.9 (3)
O3—C9—C8	103.5 (3)	N4—C52—C51	113.2 (3)
N2—C9—C25	112.0 (3)	O6—C52—C68	108.3 (3)
O3—C9—C25	107.9 (3)	N4—C52—C68	110.9 (3)

Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: AB1494). Services for accessing these data are described at the back of the journal.

References

Bock, M. G., Dipardo, R. M., Evans, B. E., Rittle, K. E., Whitter, W. L., Veber, D. F., Anderson, P. S. & Freidinger, R. M. (1989). *J. Med. Chem.* **32**, 13–16.

Bunin, B. A., Plunkett, M. J. & Ellman, J. A. (1994). *Proc. Natl Acad. Sci. USA*, **91**, 4708–4712.

Capuano, L. & Gartner, K. (1981). *J. Heterocycl. Chem.* **18**, 1341–1343.

Capuano, L. & Wamprecht, C. (1986). *Liebigs Ann. Chem.* pp. 938–943.

Meier, H., Lauer, W. & Krause, V. (1986). *Chem. Ber.* **119**, 3382–3393.

Sheldrick, G. M. (1985). *SHELXS*86. *Program for the Solution of Crystal Structures*. University of Göttingen, Germany.

Sheldrick, G. M. (1993). *SHELXL*93. *Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

Sternbach, L. H. (1979). *J. Med. Chem.* **22**, 1–7.

Xu, J.-X. & Jin, S. (1994). *Chin. Chem. Lett.* pp. 557–560.

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2,2′-Bibenzoxazole

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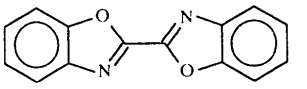
Abstract

In the title compound, $C_{14}H_8N_2O_2$, the oxazole ring systems are in a coplanar configuration. The length of the C—C bond between the benzoxazole units is 1.447 (3) Å. In the five-membered oxazole rings, C1—O = 1.345 (2) Å and C1—N = 1.289 (2) Å.

Comment

The title compound, (I), was obtained after a solution of *mer*-tris(2-trimethylsiloxyphenyl isocyanide)tricarbonylchromium in methanol was exposed to daylight for three weeks. The metal complex decomposes in methanolic solution and 2-trimethylsiloxyphenyl isocyanide is liberated; cyclization of the free ligand results in heterocyclic benzoxazole (Ferris *et al.*, 1973; Fraser *et al.*, 1985). Photodehydrodimerization of this compound yields 2,2′-bibenzoxazole (Grellmann & Tauer, 1974).



(I)

Dense packing of the molecules in the crystal structure is reflected in the stacking distance of 3.34 Å between two molecules.

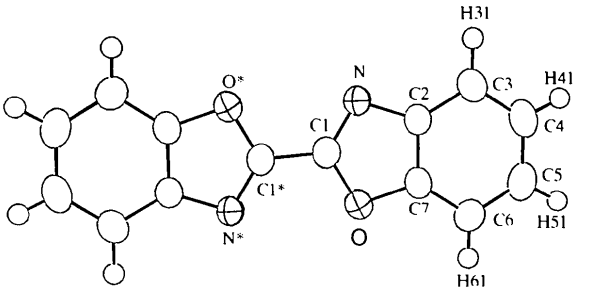


Fig. 1. Plot showing the displacement ellipsoids at the 50% probability level and the atomic numbering scheme. H atoms are shown as small spheres with arbitrary radii. Starred atoms (*) have transformed coordinates $(-x, -y, -z + 1)$.

Experimental

Crystals were grown by slow diffusion of hexane into a solution of 2,2-bibenzoxazole in chloroform.

Crystal data

$C_{14}H_8N_2O_2$
M_r = 236.23
Monoclinic
$P2_1/n$
a = 4.644 (3) Å
b = 16.559 (5) Å
c = 7.007 (3) Å
β = 94.19 (4)°
V = 537.4 (4) Å^3
Z = 2
D_x = 1.456 Mg m^{-3}
D_m = 1.460 Mg m^{-3}
D_m measured by flotation in $CHCl_3/CH_2Cl_2$
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 5.0–11.5°
μ = 0.101 mm^{-1}
T = 293 (2) K
Prism
0.61 × 0.28 × 0.28 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.027$
$\omega/2\theta$ scans	$\theta_{max} = 25°$
Absorption correction: none	$h = 0 \rightarrow 5$
1064 measured reflections	$k = 0 \rightarrow 19$
944 independent reflections	$l = -8 \rightarrow 8$
791 reflections with $I > 2\sigma(I)$	3 standard reflections every 200 reflections intensity decay: 1.8%

Refinement

Refinement on F^2	$\Delta\rho_{max} = 0.270$ e Å^{-3}
$R[F^2 > 2\sigma(F^2)] = 0.044$	$\Delta\rho_{min} = -0.186$ e Å^{-3}
$wR(F^2) = 0.133$	Extinction correction: *SHELXL*97 (Sheldrick, 1997)
$S = 1.084$	Extinction coefficient: 0.14 (2)
944 reflections	Scattering factors from *International Tables for Crystallography* (Vol. C)
99 parameters	
All H atoms refined	
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	
$(\Delta/\sigma)_{max} < 0.001$	

Table 1. *Selected geometric parameters (Å, °)*

O—C1	1.345 (2)	C3—C4	1.379 (3)
O—C2	1.381 (2)	C7—C6	1.390 (3)
N—C1	1.289 (2)	C5—C6	1.367 (3)
N—C7	1.393 (2)	C5—C4	1.384 (3)
C2—C3	1.368 (2)	C1—C1^{i}	1.447 (3)
C2—C7	1.377 (2)		
C1—O—C2	103.40 (13)	C6—C7—N	130.94 (16)
C1—N—C7	103.21 (14)	C6—C5—C4	122.51 (19)
C3—C2—C7	124.47 (17)	C5—C6—C7	116.38 (18)
C3—C2—O	128.21 (16)	N—C1—O	116.92 (15)
C7—C2—O	107.32 (15)	N—C1—C1^{i}	126.1 (2)
C2—C3—C4	114.88 (17)	O—C1—C1^{i}	117.01 (19)
C2—C7—C6	119.92 (16)	C3—C4—C5	121.83 (17)
C2—C7—N	109.14 (15)		

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1990). Cell refinement: *CAD-4 Software*. Data reduction: *MolEN* (Enraf–Nonius, 1992). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997). Molecular graphics: *ZORTEP* (Zsolnai & Pritzkow, 1995). Software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: KA1251). Services for accessing these data are described at the back of the journal.

References

Enraf–Nonius (1990). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.

Enraf–Nonius (1992). *MolEN. An Interactive Intelligent System for Crystal Structure Analysis*. Enraf–Nonius, Delft, The Netherlands.

Ferris, J. P., Antonucci, F. R. & Trimmer, R. W. (1973). *J. Am. Chem. Soc.* **95**, 919–920.

Fraser, R. R., Mansou, T. S. & Savard, S. (1985). *Can. J. Chem.* **63**, 3505–3507.

Grellmann, K. H. & Tauer, E. (1974). *Tetrahedron Lett.* **4**, 375–376.

Sheldrick, G. M. (1985). *SHELXS*86. *Program for the Solution of Crystal Structures*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXL*97. *Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

Zsolnai, L. & Pritzkow, H. (1995). *ZORTEP. ORTEP Program for Personal Computers*. University of Heidelberg, Germany.

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(2,4-Dichlorophenoxy)acetohydrazide

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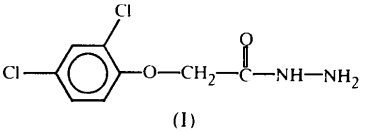
Abstract

The title compound, $C_8H_8Cl_2N_2O_2$, is an intermediate compound in the synthesis of one of the important 1,2,4-triazoles that possess diverse pharmacological activities.

Comment

Various 1,2,4-triazoles are found to possess varied pharmacological activities. Many of them are conveniently prepared starting from hydrazides. They are important due to their analgesic, antibacterial, antifungal, antiviral, herbicidal, insecticidal and antitubercular (Rudnicka & Osmialowska, 1979) properties. They also find application in the preparation of photographic plates (Martin *et al.*, 1978), in polymers and as analytical reagents for the estimation of metals such as silver, copper and lead. Various condensed nitrogen heterocycles derived from hydrazides are important due to their antibacterial and anticancer properties. The title hydrazide, (I), is an intermediate compound in the synthesis of 4-amino-3-(2,4-dichlorophenoxymethyl)-5-mercapto-1,2,4-triazole.



(I)

The bond distances and angles of (I) do not show any large deviations from expected values.