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1,1′-Bi-1*H*-benzimidazole-2,2′-dicarbaldehyde

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In the title biazole, $C_{16}H_{10}N_4O_2$, the linking N—N bond length is 1.375 (2) Å and the dihedral angle between the staggered imidazole rings is 94.6 (2)°.

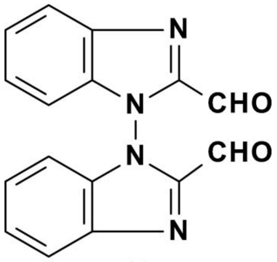
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.057
wR factor = 0.134
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.

Comment

Biazoles connected by N—N bonds are often viewed as weakly bound dimers which readily homolyse to two radicals (Zimmermann *et al.*, 1961). While this is the case for biazoles with multiple aromatic substitutents, there are now numerous examples of N—N-linked biazoles with remarkable stability and utility (Reddy *et al.*, 2002). Surprisingly few N—N-linked biimidazoles have been isolated, a trend that is due to their circuitous synthetic access (de Mendoza *et al.*, 1981). The remarkable stabililty of bibenzimidazoles and their chiral atropisomerism make them potentially useful chiral auxillaries for stereoselective transition metal catalysts, and several diphosphine derivatives and complexes have recently been prepared and structurally characterized (Benincori *et al.*, 1997). The title compound, (I), is a key synthon in the preparation of bibenzimidazole derivatives and is readily prepared by selenium dioxide oxidation of the corresponding 2,2′-dimethyl analog.



(I)

The molecular stucture of (I) is shown in Fig. 1. The N1—N3 bond length [1.372 (2) Å] is nearly identical to that in the corresponding bisdiphenylphosphino analog, in which N—N = 1.375 (2) Å for the free ligand and 1.377 (5) Å in its palladium dichloride complex (Benincori *et al.* 1997). A 2,2′-biaromatic analog has also been structurally characterized and, in this case, the N—N bond length is 1.380 (1) Å (Speier & Párkányi, 1986). In (I), the dihedral angle between the imidazole rings is 94.6 (2)°.

Experimental

The title compound was prepared according to literature methods (de Mendoza *et al.*, 1981) and large crystals were obtained by evaporation

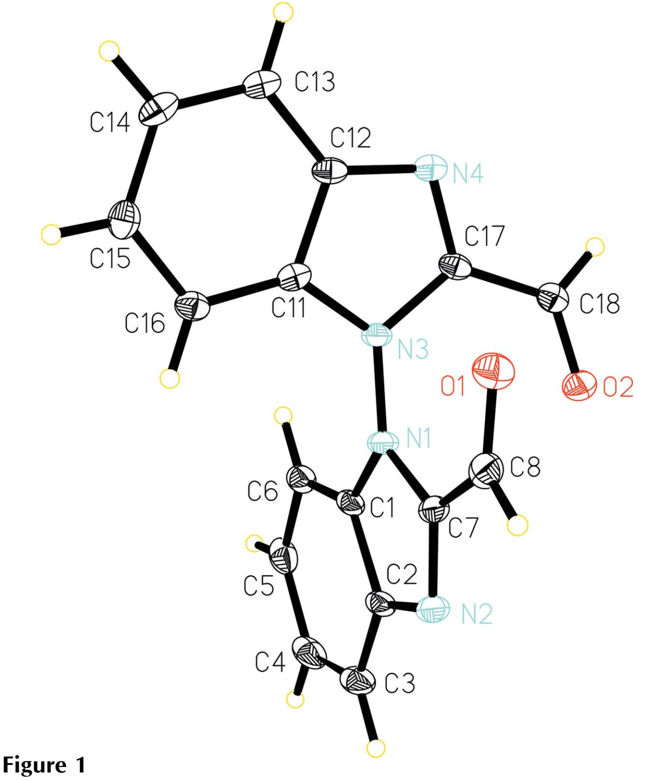


Figure 1
The molecular structure of (I), showing 45% probablilty ellipsoids.

of a chloroform solution of (I) at room temperature over the course of a week.

Crystal data

$C_{16}H_{10}N_4O_2$
$M_r = 290.28$
Triclinic, $P\bar{1}$
$a = 6.8190$ (16) Å
$b = 9.216$ (2) Å
$c = 11.619$ (3) Å
$\alpha = 68.246$ (2)°
$\beta = 76.938$ (3)°
$\gamma = 73.881$ (3)°
$V = 645.3$ (3) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 273$ (2) K
0.15 × 0.10 × 0.04 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: none
5486 measured reflections
2703 independent reflections
2178 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.134$
$S = 1.10$
2703 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max} = 0.40$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.23$ e Å^{-3}

H atoms were placed in calculated positions, with C—H = 0.93 Å, and included in the refinement in the riding-model approximation, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$

Data collection: *SMART* (Bruker, 1996); cell refinement: *SAINT* (Bruker, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1996); software used to prepare material for publication: *SHELXTL*.

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