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6,6′-Bis(2*H*-1,2,3-benzotriazol-2-yl)-4,4′-bis(2,4,4-trimethylpentan-2-yl)-2,2′-methylenebiphenol

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The complete molecule of the title compound, $C_{41}H_{50}N_6O_2$, is generated by crystallographic twofold rotation symmetry, with one C atom lying on the rotation axis. A bifurcated intramolecular O—H···(N,N) hydrogen bond helps to establish the molecular conformation.

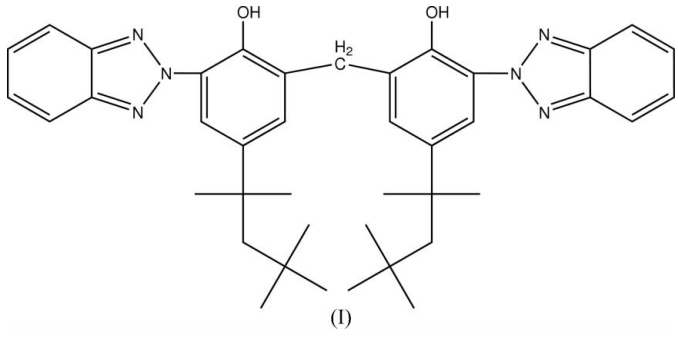
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.090
wR factor = 0.197
Data-to-parameter ratio = 15.6

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

Comment

Benzotriaaole derivatives have important applications as absorbers of ultraviolet light (Shitagaki *et al.*, 2004). As part of our studies in this area, we report here the synthesis and crystal structure of the title compound, (I) (Fig. 1).



(I)

The complete molecule of (I) is generated by crystallographic twofold rotation symmetry, with atom C15 lying on the rotation axis. The dihedral angle between the mean plane of the N2/N1/N3/C16–C21 fused ring system and that of the C9–C14 ring is 9.20 (19)°.

A bifurcated intramolecular O—H···(N,N) hydrogen bond (Table 1) helps to establish the molecular conformation.

Experimental

2-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-6-(bromomethyl)-4-(2,4,4-trimethylpentan-2-yl)phenol (10 mmol) and 2-(2*H*-benzo[*d*][1,2,3]-triazol-2-yl)-4-(2,4,4-trimethylpentan-2-yl)phenol (10 mmol) (Xing *et al.*, 2007) were reacted in benzene (100 ml) for 12 h with aluminium(III) chloride as catalyst. After cooling and filtering, the crude title compound was obtained, and this was purified by recrystallization from ethyl acetate. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{41}H_{50}N_6O_2$
M_r = 658.87
Orthorhombic, *Pbcn*
a = 18.302 (4) Å
b = 8.0960 (16) Å
c = 24.553 (5) Å
V = 3638.1 (13) Å^3
Z = 4
D_x = 1.203 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.963, T_{max} = 0.993
3587 measured reflections
3545 independent reflections
1789 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.090
$wR(F^2)$ = 0.197
S = 1.06
3545 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 1.8628P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N3	0.82	1.87	2.596 (5)	146
O1—H1···N1	0.82	2.46	2.883 (5)	113

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å and O—H = 0.82 Å, and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

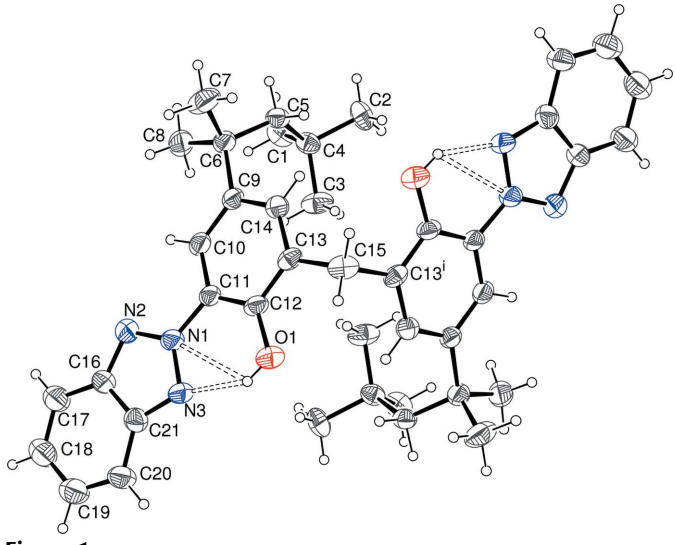


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Hydrogen bonds are indicated by double dashed lines. [Symmetry code: (i) $-x, y, \frac{1}{2} - z$.]

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