Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(2*H*-1,2,3-Benzotriazol-2-yl)-4-(2,4,4-trimethylpentan-2-yl)phenol

Zhi-Tao Xing,* Wei-Lin Ding, Pin-Liang Wang, Feng Han and Hai-Bo Wang

Department of Applied Chemistry, College of Science, Nanjing University of Technolgy, Xinmofan Road No. 5, Nanjing 210009, People's Republic of China

Correspondence e-mail: wanghaibo@njut.edu.cn

Received 27 November 2006
Accepted 27 November 2006

Key indicators

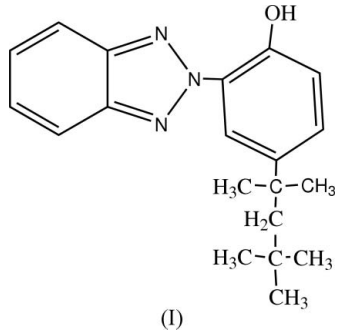
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.063
wR factor = 0.137
Data-to-parameter ratio = 9.1

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

In the title compound, $C_{20}H_{25}N_3O$, an intramolecular O—H···N hydrogen bond helps to establish the molecular conformation.

Comment

Benzotriaaole derivatives have important applications as ultraviolet absorbers (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 dihedral angle between the mean plane of the N2/N1/N3/C20/C15 ring and that of the C9-containing ring is 9.20 (19)°. An intramolecular O—H···N hydrogen bond (Table 1) helps to establish the molecular conformation.

Experimental

2-Nitroaniline, diazotized sodium nitrite and 4-(2,4,4-trimethylpentan-2-yl)phenol were reacted in a 1:1.05:1 ratio in the presence of hydrochloric acid to produce 2-[(2-nitrophenyl)diazenyl]-4-(2,4,4-trimethylpentan-2-yl)phenol, (II). Compound (II) (1 mol) was then

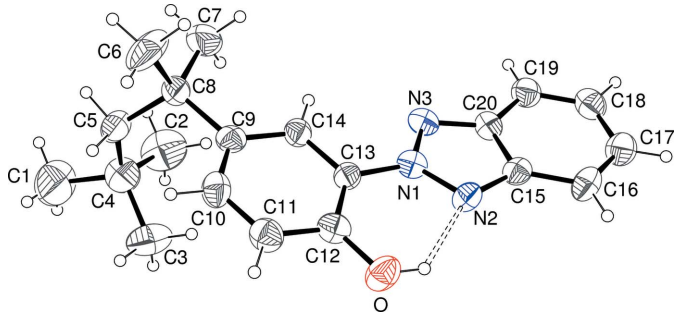


Figure 1
The molecular structure of (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). The hydrogen bond is indicated by a dashed line.

reduced with hydrazine hydrate (2 mol) to produce 2-(2*H*-1,2,3-benzotriazol-2-yl)-4-(2,4,4-trimethylpentan-2-yl)phenol *N*-oxide, (III). Finally, (III) (1 mol) was reduced with zinc powder (1.5 mol) to produce the title compound, (I). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{20}H_{25}N_3O$
M_r = 323.43
Orthorhombic, $Pca2_1$
a = 13.177 (3) Å
b = 16.289 (3) Å
c = 8.4280 (17) Å
V = 1809.0 (6) Å^3
Z = 4
D_x = 1.188 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
Block, colourless
0.40 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.971, T_{max} = 0.993
1916 measured reflections
1916 independent reflections
937 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.137
S = 0.95
1916 reflections
211 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0376P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O—H1···N2	0.85	1.97	2.618 (6)	132

All H atoms were placed in calculated positions (C—H = 0.93–0.97 Å and O—H = 0.85 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: *PLATON* (Spek, 2003).

References

Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Shitagaki, S., Seo, S. & Nishi, T. (2004). PCT Int. Appl. WO 2004060021.
Siemens (1996). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.