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Key indicators

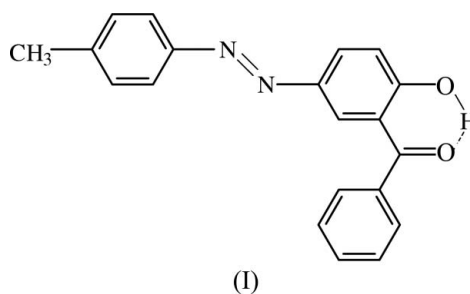
Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.040
 wR factor = 0.115
Data-to-parameter ratio = 14.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**(E)-2-Benzoyl-4-[(4-methylphenyl)diazenyl]-phenol**

The title compound, $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_2$, displays a *trans* configuration with respect to the $\text{N}=\text{N}$ double bond. The aromatic rings bridged by the azo group are nearly coplanar, forming a dihedral angle of $6.83(8)^\circ$. A strong intramolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond is observed. In the three-dimensional network, the molecules are linked by weak van der Waals interactions.

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Comment

The azo compound class accounts for 60–70% of all dyes. These compounds are widely used in the textile, printing, paper manufacturing, pharmaceutical and food industries. All of them contain at least one azo group ($-\text{N}=\text{N}-$) which links two sp^2 -hybridized C atoms. During the course of our studies aimed at the synthesis and characterization of new azo compounds, the title compound, (I), was isolated. We report here the crystal structure of (I).



In the azo group of (I), the $\text{N1}-\text{C5}$ and $\text{N2}-\text{C8}$ bond lengths indicate significant single-bond character, whereas the $\text{N1}-\text{N2}$ bond length is indicative of significant double-bond character (Table 1). The benzene rings $\text{C2}-\text{C7}$ and $\text{C8}-\text{C13}$ adopt a *trans* configuration about the azo group, and are essentially coplanar, forming a dihedral angle of $6.83(8)^\circ$. The dihedral angle between the $\text{C8}-\text{C13}$ and $\text{C15}-\text{C20}$ aromatic rings is $58.97(8)^\circ$. A strong intramolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond is observed (Table 2). In the crystal structure, the molecules are linked by weak van der Waals interactions.

Experimental

A mixture of 4-methylaniline (0.54 g, 5 mmol), water (20 ml) and concentrated hydrochloric acid (1.25 ml, 15 mmol) was stirred until a clear solution was obtained. This solution was cooled to 273–278 K and a solution of sodium nitrite (0.41 g, 7 mmol) in water was added dropwise while the temperature was maintained below 278 K. The resulting mixture was stirred for 30 min in an ice bath. 2-Hydroxybenzophenone (1 g, 5 mmol) solution (pH 9) was gradually added to

a cooled solution of 4-methylbenzenediazonium chloride, prepared as described above, and the resulting mixture was stirred at 273–278 K for 60 min in an ice bath. The product was recrystallized from ethyl alcohol to obtain the solid title compound. Crystals suitable for X-ray analysis were obtained after 1 d by slow evaporation of an ethanol solution (yield 25%; m.p. 406–408 K).

Crystal data

C₂₀H₁₆N₂O₂
M_r = 316.35
 Monoclinic, *P*2₁/*c*
a = 15.6711 (13) Å
b = 5.8068 (2) Å
c = 18.7764 (13) Å
 β = 111.706 (6)°
V = 1587.48 (18) Å³
Z = 4

D_x = 1.324 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 17500 reflections
 θ = 2.2–27.9°
 μ = 0.09 mm⁻¹
T = 293 (2) K
 Prism, brown
 0.66 × 0.46 × 0.20 mm

Data collection

Stoe IPDS-2 diffractometer
 ω scans
 Absorption correction: integration
 (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.953, *T_{max}* = 0.984
 15552 measured reflections
 3115 independent reflections

2171 reflections with *I* > 2σ(*I*)
R_{int} = 0.038
 θ_{max} = 26.0°
h = -19 → 19
k = -7 → 7
l = -22 → 22

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.040
wR(*F*²) = 0.115
S = 1.02
 3115 reflections
 217 parameters
 H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0643*P*)² + 0.0625*P*]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.17 e Å⁻³
 Δρ_{min} = -0.13 e Å⁻³

Table 1

Selected bond lengths (Å).

N1–N2	1.2522 (18)	N2–C8	1.423 (2)
N1–C5	1.424 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O1–H1···O2	0.82	1.84	2.5608 (17)	146

All H atoms were placed in calculated positions and refined using a riding model, with C–H = 0.93–0.96 Å, O–H = 0.82 Å and *U*_{iso}(H) = 1.2–1.5*U*_{eq}(parent atom).

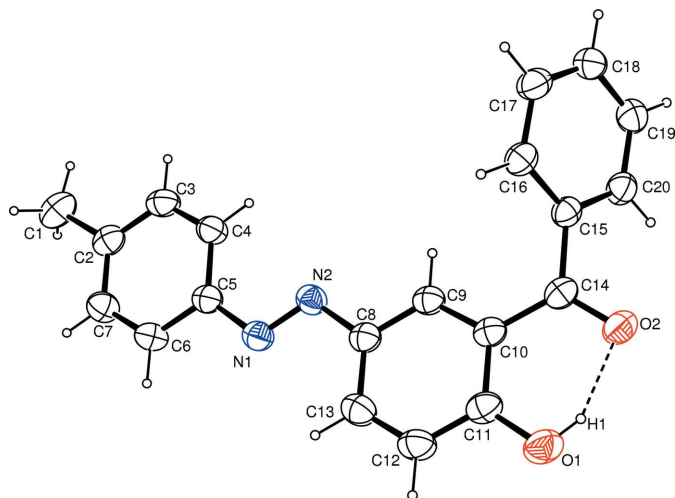


Figure 1

A view of the molecular structure of (I). The intramolecular O–H···O hydrogen bond is indicated by a dashed line.

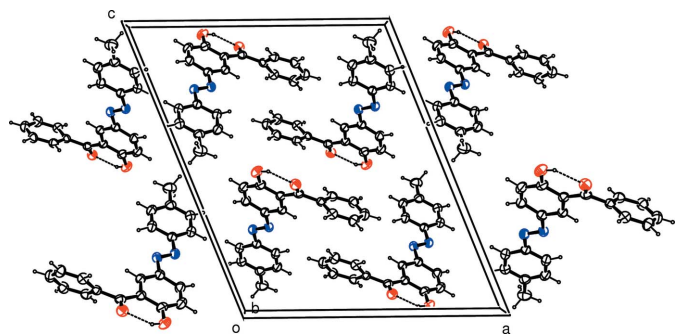


Figure 2

Packing diagram of (I), viewed along the *b* axis. Intramolecular O–H···O hydrogen bonds are shown as dashed lines.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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