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N,*N*,*N*′,*N*′-Tetrakis{3-[1-(2-hydroxy-4-methoxyphenyl)ethenylamino]propyl}ethylenediamine

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.058
wR factor = 0.175
Data-to-parameter ratio = 14.4

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

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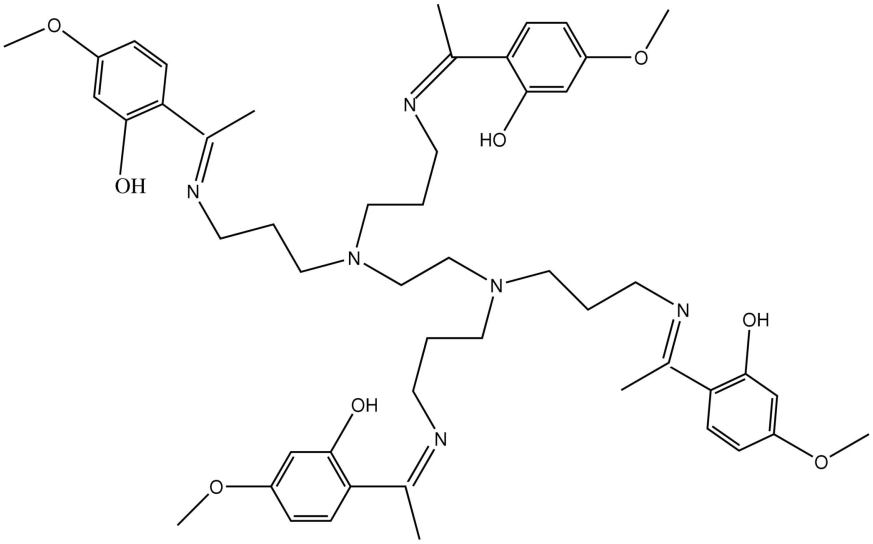
The title compound, $C_{50}H_{68}N_6O_8$, is a new Schiff base compound synthesized by the condensation reaction of paeonol and *N*,*N*,*N*′,*N*′-tetrakis(3-aminopropyl)ethylenediamine in absolute methanol. The molecule possesses a crystallographically imposed centre of symmetry and demonstrates normal values of bond lengths and angles.

Comment

1-Aceto-4-methoxyphenol (common name paeonol) is an effective component of many traditional Chinese medicines, and its ramifications derivatives have attracted considerable attention because of their potential biological properties. As part of our ongoing study of Schiff base compounds of paeonol (Xu *et al.*, 2006), we present here the crystal structure of the title compound, (I), a new Schiff base compound synthesized by the condensation reaction of paeonol and *N*,*N*,*N*′,*N*′-tetrakis(3-aminopropyl)ethylenediamine, which has itself been studied extensively (Mikuriya *et al.*, 1985; Micheloni *et al.*, 1986).



(I)

The molecule of (I) possesses a crystallographically imposed centre of symmetry (Fig. 1). All bond lengths and angles are normal (Allen *et al.*, 1987). The C9—N2 and C18—N3 bond lengths of 1.290 (4) and 1.302 (4) Å, respectively, are typical for C═N Schiff base bonds. The benzene rings C10–C15 and C19–C24 make a dihedral angle of 73.94 (1)°. Intramolecular O—H···N hydrogen bonds (Table 1) influence the molecular geometry.

Experimental

To a stirred solution of paeonol (0.664 g, 4 mmol) in absolute methanol (25 ml) was added dropwise a solution of *N*,*N*,*N*′,*N*′-tetrakis(3-aminopropyl)ethylenediamine (0.288 g, 1.0 mmol) in absolute methanol (10 ml) at room temperature. After stirring for 3 h at 320 K, the precipitate was filtered off. Single crystals of (I) were obtained by slow evaporation of the filtrate after 5 d.

Crystal data

$C_{50}H_{68}N_6O_8$
M_r = 881.10
Triclinic, $P\overline{1}$
a = 6.761 (4) Å
b = 11.928 (6) Å
c = 15.575 (8) Å
α = 82.263 (8)°
β = 85.777 (8)°
γ = 73.743 (8)°
V = 1194.1 (11) Å^3
Z = 1
D_x = 1.225 Mg m^{-3}
Mo *Kα* radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
Block, yellow
0.25 × 0.17 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{\min}$ = 0.980, $T_{\max}$ = 0.993
6277 measured reflections
4159 independent reflections
1704 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.034
$\theta_{\max}$ = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.175
S = 0.99
4159 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 0.24 e Å^{-3}
$\Delta\rho_{\min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.82	1.74	2.477 (4)	149
O3—H3···N3	0.82	1.75	2.484 (4)	149

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and torsion angles were refined to fit the electron density, with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C). Hydroxy H atoms were positioned geometrically, with O—H = 0.82 Å, and refined in riding mode, with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(O). Other H atoms were positioned geometrically, with C—H = 0.93 (aromatic) and 0.97 Å (methylene), and refined in riding mode, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

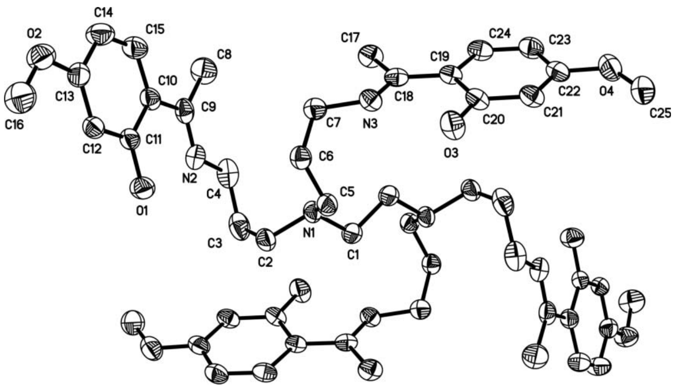


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and atom numbering. Unlabelled atoms are related to the labelled atoms by the symmetry operation $(1 - x, 1 - y, 1 - z)$. H atoms have been omitted for clarity.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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