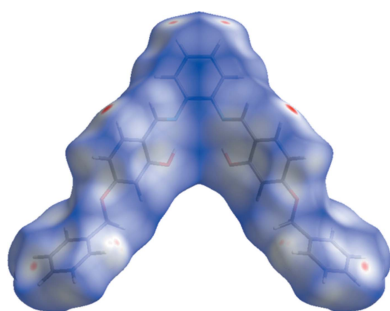# research communications

Crystal structure, Hirshfeld surface analysis and antioxidant capacity of 2,2'-{(1*E*,1'*E*)-[1,2-phenylenebis(azanylylidene)]bis(methanylylidene)}bis(5-benzyloxy)phenol

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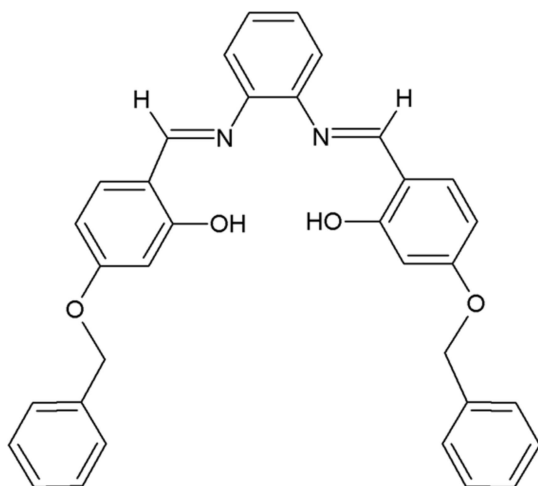
The whole molecule of the title Schiff base compound, $C_{34}H_{28}N_2O_4$, is generated by mirror symmetry, with the mirror bisecting the central benzene ring. It was synthesized *via* the condensation reaction of 1,2-diaminebenzene with 4-benzyloxy-2-hydroxybenzaldehyde. The molecule is V-shaped and there are two intramolecular O—H⋯N hydrogen bonds present forming $S(6)$ ring motifs. The configuration about the C=N imine bonds is *E*. The central benzene ring makes dihedral angles of 41.9 (2) and 43.6 (2)° with the phenol ring and the outer benzyloxy ring, respectively. The latter two rings are inclined to each other by 84.4 (2)°. In the crystal, molecules are linked by C—H⋯π interactions, forming layers lying parallel to the *ab* plane. The Hirshfeld surface analysis and the two-dimensional fingerprint plots confirm the predominance of these interactions in the crystal structure. The antioxidant capacity of the compound was determined by the cupric reducing antioxidant capacity (CUPRAC) process.

1. Chemical context

Schiff base derivatives are a biologically versatile class of compounds possessing diverse activities, such as anti-oxidant (Haribabu *et al.*, 2015, 2016), anti-inflammatory (Alam *et al.*, 2012), antianxiety, antidepressant (Jubie *et al.*, 2011), anti-tumour, antibacterial, and fungicidal properties (Refat *et al.*, 2008; Kannan & Ramesh, 2006). Bis-bidentate Schiff base ligands have been studied extensively and used as building blocks in metallo-supramolecular chemistry (Birkedal & Pattison, 2006; Shahverdizadeh & Tiekink, 2011; Chu & Huang, 2007; Yoshida & Ichikawa, 1997; Kruger *et al.*, 2001). The common structural feature of these compounds is the presence of an azomethine group, linked by a η methylene bridge, which can act as a hydrogen-bond acceptor. In view of this interest we have synthesized the title compound, (I), and report herein on its crystal structure. The ^{1}H NMR NMR spectrum reveals the presence of an imino group (N=CH) in the range δ = 8.5–8.7 p.p.m. The antioxidant capacity of the compound was determined by the cupric reducing antioxidant capacity (CUPRAC) process.

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

$Cg2$ is the centroid of the C5–C10 phenol ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···N1	0.82	1.90	2.622 (5)	147
C2—H2···$Cg2^i$	0.93	2.88	3.499 (5)	125
C13—H13···$Cg2^{ii}$	0.93	2.60	3.493 (5)	161

Symmetry codes: (i) $x, -y + 1, z - \frac{1}{2}$; (ii) $x, -y, z + \frac{1}{2}$.

2. Structural commentary

The molecular structure of compound (I) is illustrated in Fig. 1. The asymmetric unit consists of half a molecule, with the whole molecule being generated by mirror symmetry. The mirror bisects the central benzene ring, *viz.* bonds C1—C1^i and C3—C3^i [symmetry code: (i) $-x, y, z$]. In the molecule there are two intramolecular O—H···N hydrogen bonds present (Table 1), which form $S(6)$ ring motifs as shown in Fig. 1. The configuration of the C4=N1 imine bonds is *E* and the C4=N1 bond length is 1.278 (6) Å. The C3—N1=C4 bond angles are less than 120° [118.9 (4)°], and the imine group has a C3—N1—C4—C5 torsion angle of −176.8 (4)°. The molecule is V-shaped and the two arms are non-planar; the central benzene ring forms dihedral angles of 41.9 (2) and
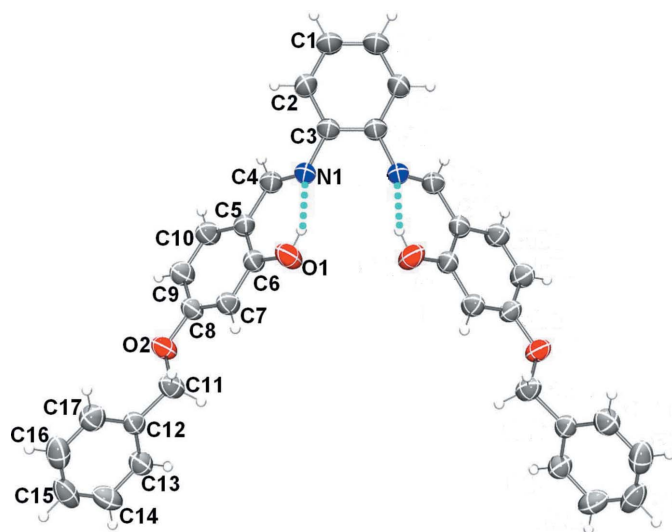
43.6 (2)° with the phenol ring (C5-C10) and the outer benzyloxy ring (C12–C17), respectively. The latter two rings are almost normal to each other, with a dihedral angle of 84.4 (2)°.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal of (I), molecules are linked by C—H···π interactions (Table 1), forming layers parallel to the (001) plane, as illustrated in Fig. 2.

The Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) and the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were performed with *Crystal-Explorer17* (Turner *et al.*, 2017). The Hirshfeld surface of compound (I) mapped over d_{norm} is given in Fig. 3, and the fingerprint plots are given in Fig. 4. They reveal that the principal intermolecular interactions are H···H at 45.7% (Fig. 4*b*) and H···C/C···H at 34.6% (Fig. 4*c*), followed by the H···O/O···H interactions at 13.6% (Fig. 4*d*).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.39, last update February 2018; Groom *et al.*, 2016) for similar compounds yielded four hits. These compounds (see Fig. 5) include 5,5′-dihydroxy-2,2′-[*o*-phenylenebis(nitrilomethylene)]diphenol ethanol solvate (II) (CSD refcode HUVXUT; Soroceanu *et al.*, 2013), 5,5′-dimethoxy-2,2′-[4,5-dimethyl-*o*-phenylenebis(nitrilomethylidyne)]di-

Figure 1
View of the molecular structure of compound (I), with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the mirror symmetry code: (i) $-x, y, z$. The intramolecular O—H···N hydrogen bonds (see Table 1) are shown as dashed lines.
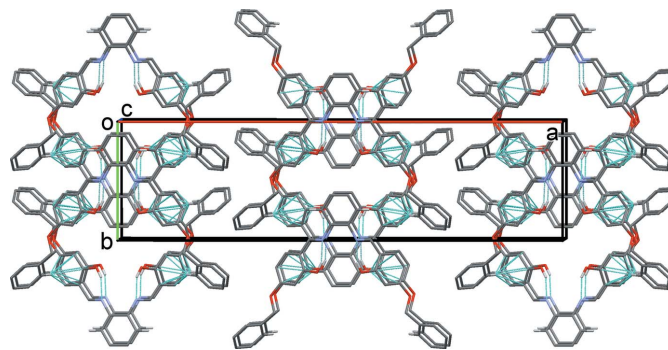

Figure 2
Crystal packing of compound (I) viewed along the *c* axis, with the O—H···N intramolecular hydrogen bonds and the C—H···π interactions (see Table 1) illustrated as dashed lines.
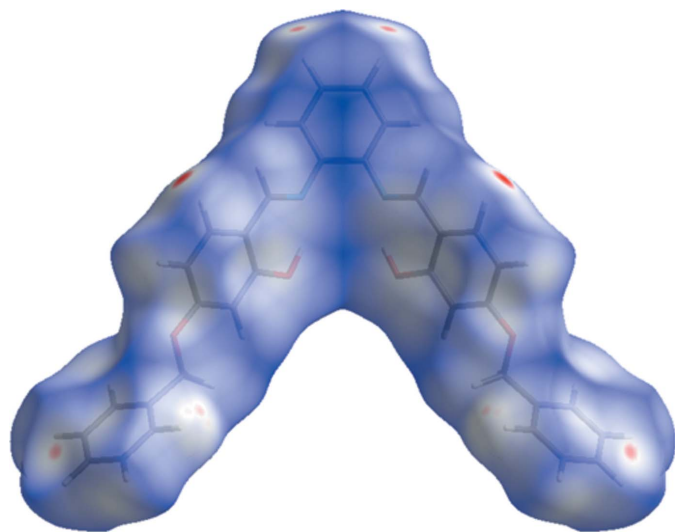
Figure 3
View of the Hirshfeld surface of (I) mapped over d_{norm}.

phenol (III) (KUSJIS; Kargar *et al.*, 2010), 1,2-bis{[(2-hy-droxy-4-methoxyphenyl)(phenyl)methylene]amino}benzene (IV) (SOXCIS; Lippe *et al.*, 2009) and 5,5′-dimethoxy-2,2′-1,2-phenylenebis(nitrilomethylidyne)]diphenol (V) (XIFREK; Eltayeb *et al.*, 2007). In all four compounds there are two intramolecular O—H⋯N hydrogen bonds present forming $S(6)$ ring motifs.

In (II) the phenol rings are inclined to the central benzene ring by 53.9 (3) and 4.0 (2)° and to each other by 49.9 (2)°. In (III) the corresponding dihedral angles are 48.12 (8), 21.44 (8) and 47.70 (8)°, while in (V) the corresponding dihedral angles
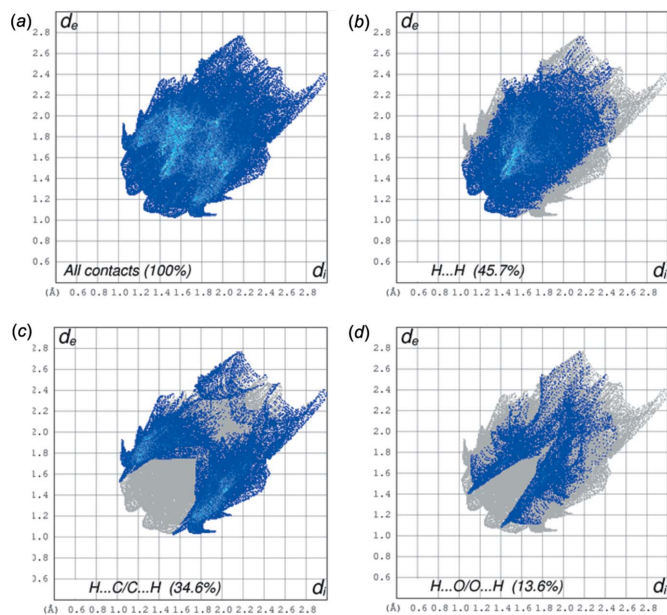

Figure 4
The two-dimensional fingerprint plots of (I): (*a*) all interactions; (*b*) H⋯H; (*c*) H⋯C/C⋯H; (*d*) H⋯O/O⋯H.
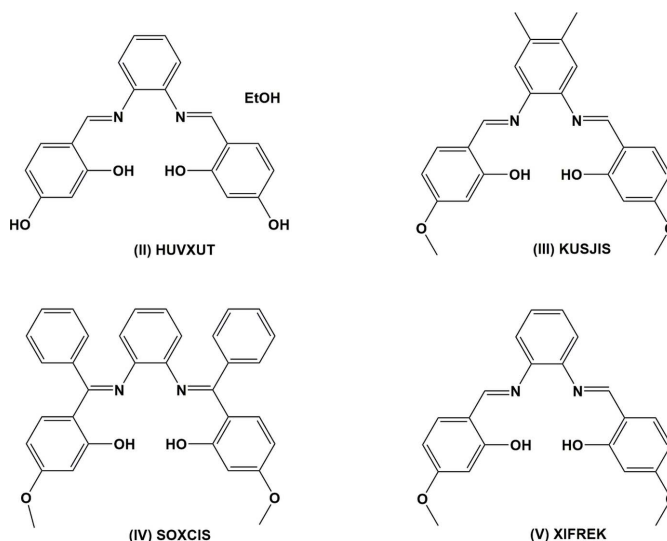

Figure 5
Similar compounds to that of the title compound, (I), in the CSD; see Section 4, *Database survey*.

are 58.29 (12), 2.20 (12) and 57.60 (12)°. In compound (IV), that possesses twofold rotational symmetry with the twofold axis bisecting the central benzene ring, the phenol rings are inclined to the central benzene ring by 82.30 (5)° and to each other by 63.76 (5)°. In the title compound, which possesses mirror symmetry, the corresponding dihedral angles are 41.9 (2) and 68.9 (2)°.

A search of the CSD for metal complexes of compounds similar to compound (I) gave over 30 hits. The ligands always coordinate in a tetradentate manner. For example, there were 13 hits for transition metal complexes of compound (II). The majority involve square-planar coordinated metal atoms, such as in complexes (5,5′-dihydroxy-2,2′-[o-phenylenebis(nitrilo-methylidyne)]diphenolato)nickel(II) dihydrate (POFFOG; Fun *et al.*, 2008) and (4,4′-{1,2-phenylenebis[(nitrilo-κN)-methylylidene]}dibenzene-1,3-diolato-κO^3)copper(II) methanol solvate (DUQBEX; Niu *et al.*, 2010). For compound (V), five hits were found; they include three sixfold-coordinated tin complexes (DOSCOF, DOSDAS, DOSFOI; Muñoz-Flores *et al.*, 2014) and two square-pyramidal manganese complexes (ODESEY, Ghaemi *et al.*, 2016; XIYQOM, Eltayeb *et al.*, 2008).

5. Antioxidant activity

The antioxidant activity profile of the synthesized compound (I) was determined by utilizing the copper(II)–neocuprine [Cu^{II}-Nc] (CUPRAC) method (Apak *et al.*, 2004). The CUPRAC method (Fig. 6) (cupric ion reducing antioxidant capacity) is based on the follow-up of the decrease in the increased absorbance of the neocuproene (Nc), copper (Cu^{+2})Nc$_2$–Cu^{+2} complex. Indeed, in the presence of an antioxidant agent, the copper–neocuproene complex is reduced and this reaction is quantified spectrophotometrically at a wavelength of 450 nm.

Table 2
Cupric ion reducing antioxidant capacity of compound (I).

	Percentage (%) Inhibition							
	12.5 µg	25 µg	50 µg	100 µg	200 µg	400 µg	800 µg	A0.50 (μg ml^{-1})
Compound (I)	0.39±0.01	0.59±0.01	0.91±0.03	1.42±0.02	1.84±0.36	3.12±0.25	4.29±0.11	15.03±1.50
BHT	1.41±0.03	2.22±0.05	2.42±0.02	2.50±0.01	2.56±0.05	2.86±0.07	3.38±0.13	8.97±3.94

According to the cupric ion reducing antioxidant capacity assay, the title compound displayed activity with variable potency in all tested concentrations, because the percentage (%) inhibition in the CUPRAC assay is good [$A_{0.50}$ = 15.03 ± 1.50 for a 4 mg dosage, compared to the results for buthylated toluene (BHT) [$A_{0.50}$ = 8.97 ± 3.94], used as a positive control (see Table 2). Note: In CUPRAC antioxidant activity, the values expressed are the mean ± s.u.s of three parallel measurements ($p < 0.05$).

6. Synthesis and crystallization

1,2-Diaminebenzene (0.027 g) and 4-benzyloxy-2-hydroxy-benzaldehyde (0.1141 g) in ethanol (15 ml) were refluxed for 1 h, then the solvent was evaporated *in vacuo*. The residue was recrystallized from ethanol, yielding yellow block-like crystals of the title compound on slow evaporation of the solvent. The purity of the compound was characterized by its NMR spectrum (250 MHz, CDCl$_3$). The azomethine proton appears in the 8.5–8.7 p.p.m. range, while the imine bond is characterized in the ^{13}C RMN spectrum with the imine C and OH signals in the range 162.23–163.34 p.p.m. ^{1}H NMR: δ = 6.5–7.6 (*m*, 12H; *H-ar*), δ = 13.7 (*s*, 1H; *OH*), δ = 5.1 (*s*, 1H; *CH$_2$*–O). ^{13}C NMR: 70.15, 120.33, 127.30, 127.64, 128.26, 128.75, 142.32, 162.23, 163.33, 163.34.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The hydroxyl H atom was located in a difference-Fourier map and initially freely refined. In the final cycles of refinements it was positioned geometrically (O—H = 0.82 Å) and refined as riding with $U_{iso}(H) =$ 1.5U_{eq}(O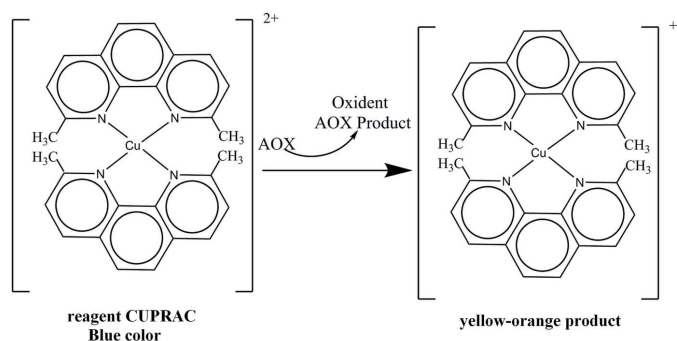). The C-bound H atoms were positioned geometrically (C–H = 0.93–0.97 Å) and refined as riding with $U_{iso}(H)$ = 1.2U_{eq}(C).

References

Alam, M. S., Choi, J.-H. & Lee, D.-U. (2012). *Bioorg. Med. Chem.* **20**, 4103–4108.
Apak, R., Güçlü, K., Özyürek, M. & Karademir, S. E. (2004). *J. Agric. Food Chem.* **52**, 7970–7981.
Birkedal, H. & Pattison, P. (2006). *Acta Cryst.* **C62**, o139–o141.
Bruker (2011). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsion, USA.
Chu, Z. & Huang, W. (2007). *J. Mol. Struct.* **837**, 15–22.
Eltayeb, N. E., Teoh, S. G., Chantrapromma, S., Fun, H.-K. & Adnan, R. (2008). *Acta Cryst.* E**64**, m670–m671.
Eltayeb, N. E., Teoh, S. G., Chantrapromma, S., Fun, H.-K. & Ibrahim, K. (2007). *Acta Cryst.* E**63**, o3094–o3095.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{34}H_{28}N_2O_4$
M_r	528.58
Crystal system, space group	Orthorhombic, $Cmc2_1$
Temperature (K)	293
a, b, c (Å)	35.297 (3), 9.3902 (6), 8.3603 (5)
V (Å^3)	2771.0 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.03 × 0.02 × 0.01
Data collection	
Diffractometer	Bruker APEXII CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4493, 2516, 1691
R_{int}	0.042
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.053, 0.158, 1.02
No. of reflections	2516
No. of parameters	185
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.24

Computer programs: *APEX2* and *SAINT* (Bruker, 2011), *SHELXT2017* (Sheldrick, 2015*a*), *SHELXL2017* (Sheldrick, 2015*b*), *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*2008) and *PLATON* (Spek, 2009).

Figure 6
Reduction of the chromogenic complex of Cu^{+2}–Nc

Fun, H.-K., Kia, R., Mirkhani, V. & Zargoshi, H. (2008). *Acta Cryst.* E**64**, m1181–m1182.

Ghaemi, A., Keyvani, B., Rayati, S., Zarei, S. & Notash, B. (2016). *Zh. Strukt. Khim. (Russ. J. Struct. Chem.)*, **57**, 1027–1030.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Haribabu, J., Subhashree, G. R., Saranya, S., Gomathi, K., Karvembu, R. & Gayathri, D. (2015). *J. Mol. Struct.* **1094**, 281–291.

Haribabu, J., Subhashree, G. R., Saranya, S., Gomathi, K., Karvembu, R. & Gayathri, D. (2016). *J. Mol. Struct.* **1110**, 185–195.

Jubie, S., Sikdar, P., Antony, S., Kalirajan, R., Gowramma, B., Gomathy, S. & Elango, K. (2011). *Pak. J. Pharm. Sci.* **24**, 109–112.

Kannan, M. & Ramesh, R. (2006). *Polyhedron*, **25**, 3095–3103.

Kargar, H., Kia, R., Khan, I. U., Sahraei, A. & Aberoomand Azar, P. (2010). *Acta Cryst.* E**66**, o728.

Kruger, P. E., Martin, N. & Nieuwenhuyzen, M. (2001). *J. Chem. Soc. Dalton Trans.* pp. 1966–1970.

Lippe, K., Gerlach, D., Kroke, E. & Wagler, J. (2009). *Organometallics*, **28**, 621–629.

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.

McKinnon, J. J., Jayatilaka, D. & Spackman, M. A. (2007). *Chem. Commun.* pp. 3814–3816.

Muñoz-Flores, B. M., Santillán, R., Farfán, N., Álvarez-Venicio, V., Jiménez-Pérez, V. M., Rodríguez, M., Morales-Saavedra, O. G., Lacroix, P. G., Lepetit, C. & Nakatani, K. (2014). *J. Organomet. Chem.* **769**, 64–71.

Niu, M., Fan, S., Liu, K., Cao, Z. & Wang, D. (2010). *Acta Cryst.* E**66**, m77.

Refat, M. S., El-Korashy, S. A., Kumar, D. N. & Ahmed, A. S. (2008). *Spectrochim. Acta Part A*, **70**, 898–906.

Shahverdizadeh, G. H. & Tiekink, E. R. T. (2011). *Acta Cryst.* E**67**, o798.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015a). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015b). *Acta Cryst.* C**71**, 3–8.

Soroceanu, A., Shova, S., Cazacu, M., Balan, I., Gorinchoy, N. & Turta, C. (2013). *J. Chem. Crystallogr.* **43**, 310–318.

Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm*, **11**, 19–32.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *CrystalExplorer17. University of Western Australia.* http://hirshfeldsurface.net

Yoshida, N. & Ichikawa, K. (1997). *Chem. Commun.* pp. 1091–1092.

Crystal structure, Hirshfeld surface analysis and antioxidant capacity of 2,2′-{(1*E*,1′*E*)-[1,2-phenylenebis(azanylylidene)]bis(methanylylidene)}bis(5-benzyloxy)phenol

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Computing details

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2011); data reduction: *SAINT* (Bruker, 2011); program(s) used to solve structure: SHELXT2017 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015b); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

2,2′-{(1*E*,1′*E*)-[1,2-Phenylenebis(azanylylidene)]bis(methanylylidene)}bis(5-benzyloxy)phenol

Crystal data

$C_{34}H_{28}N_2O_4$	$F(000) = 1112$
$M_r = 528.58$	$D_x = 1.267$ Mg m^{-3}
Orthorhombic, $Cmc2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: C 2c -2	Cell parameters from 1621 reflections
$a = 35.297$ (3) Å	$\theta = 2.2$–21.3°
$b = 9.3902$ (6) Å	$\mu = 0.08$ mm^{-1}
$c = 8.3603$ (5) Å	$T = 293$ K
$V = 2771.0$ (3) Å^3	Block, yellow
$Z = 4$	$0.03 \times 0.02 \times 0.01$ mm

Data collection

Bruker APEXII CCD diffractometer	1691 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.042$
Detector resolution: 18.4 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 3.7°$
φ and ω scans	$h = -45 \rightarrow 40$
4493 measured reflections	$k = -12 \rightarrow 5$
2516 independent reflections	$l = -10 \rightarrow 6$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.053$	Hydrogen site location: mixed
$wR(F^2) = 0.158$	H-atom parameters constrained
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.0817P)^2]$
2516 reflections	where $P = (F_o^2 + 2F_c^2)/3$
185 parameters	$(\Delta/\sigma)_{max} < 0.001$
1 restraint	$\Delta\rho_{max} = 0.29$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.05052 (9)	0.2350 (3)	0.3234 (5)	0.0693 (13)
O2	0.15676 (8)	0.0288 (3)	0.5919 (4)	0.0546 (9)
N1	0.03881 (9)	0.5084 (4)	0.3640 (5)	0.0487 (10)
C1	0.01955 (13)	0.8879 (4)	0.2654 (7)	0.0639 (15)
C2	0.03890 (12)	0.7645 (4)	0.2985 (6)	0.0567 (14)
C3	0.01982 (11)	0.6379 (4)	0.3322 (5)	0.0481 (11)
C4	0.06841 (12)	0.5103 (4)	0.4519 (6)	0.0495 (14)
C5	0.09057 (11)	0.3828 (4)	0.4833 (5)	0.0454 (11)
C6	0.08042 (11)	0.2506 (4)	0.4207 (5)	0.0475 (11)
C7	0.10168 (11)	0.1285 (4)	0.4566 (5)	0.0488 (11)
C8	0.13349 (11)	0.1401 (4)	0.5523 (5)	0.0463 (12)
C9	0.14420 (12)	0.2710 (4)	0.6146 (6)	0.0560 (16)
C10	0.12269 (12)	0.3889 (4)	0.5813 (5)	0.0560 (16)
C11	0.14781 (12)	−0.1086 (4)	0.5260 (6)	0.0547 (16)
C12	0.17886 (11)	−0.2104 (4)	0.5695 (5)	0.0449 (11)
C13	0.17544 (12)	−0.2993 (4)	0.6998 (6)	0.0543 (16)
C14	0.20330 (16)	−0.3988 (4)	0.7345 (6)	0.0677 (17)
C15	0.23502 (14)	−0.4070 (5)	0.6404 (7)	0.0700 (19)
C16	0.23920 (14)	−0.3165 (6)	0.5124 (7)	0.0697 (17)
C17	0.21118 (13)	−0.2190 (5)	0.4765 (6)	0.0617 (17)
H1	0.03276	0.97121	0.24301	0.0770*
H1O	0.04038	0.31254	0.30933	0.1040*
H2	0.06524	0.76529	0.29851	0.0680*
H4	0.0777 (10)	0.604 (4)	0.509 (5)	0.041 (9)*
H7	0.09442	0.04030	0.41635	0.0580*
H9	0.16571	0.27872	0.67824	0.0670*
H10	0.12968	0.47594	0.62529	0.0670*
H11A	0.12385	−0.14214	0.56862	0.0660*
H11B	0.14557	−0.10203	0.41061	0.0660*
H13	0.15420	−0.29259	0.76516	0.0650*
H14	0.20047	−0.45974	0.82141	0.0810*
H15	0.25371	−0.47378	0.66311	0.0840*
H16	0.26095	−0.32099	0.44979	0.0840*
H17	0.21407	−0.15860	0.38915	0.0740*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0640 (19)	0.0400 (16)	0.104 (3)	0.0056 (14)	−0.0359 (19)	−0.0063 (17)
O2	0.0595 (17)	0.0386 (14)	0.0658 (17)	0.0080 (12)	−0.0166 (15)	−0.0028 (14)

N1	0.0416 (17)	0.0335 (16)	0.071 (2)	0.0021 (14)	0.0019 (18)	0.0024 (15)
C1	0.063 (3)	0.0317 (19)	0.097 (3)	−0.0042 (16)	−0.001 (3)	0.003 (2)
C2	0.047 (2)	0.041 (2)	0.082 (3)	−0.0048 (17)	−0.002 (2)	0.000 (2)
C3	0.049 (2)	0.0322 (18)	0.063 (2)	0.0022 (16)	0.002 (2)	−0.0028 (17)
C4	0.049 (2)	0.0345 (19)	0.065 (3)	0.0002 (17)	0.003 (2)	−0.0024 (18)
C5	0.042 (2)	0.0373 (19)	0.057 (2)	−0.0015 (16)	0.002 (2)	−0.0033 (18)
C6	0.042 (2)	0.0364 (19)	0.064 (2)	−0.0017 (16)	−0.008 (2)	−0.0015 (17)
C7	0.051 (2)	0.0365 (18)	0.059 (2)	−0.0007 (16)	−0.010 (2)	−0.0041 (19)
C8	0.047 (2)	0.039 (2)	0.053 (2)	0.0063 (16)	−0.0047 (19)	0.0005 (17)
C9	0.058 (3)	0.045 (2)	0.065 (3)	−0.0010 (18)	−0.017 (2)	−0.003 (2)
C10	0.060 (3)	0.039 (2)	0.069 (3)	−0.0035 (18)	−0.011 (2)	−0.006 (2)
C11	0.059 (3)	0.041 (2)	0.064 (3)	0.0043 (19)	−0.013 (2)	−0.0047 (19)
C12	0.043 (2)	0.0378 (19)	0.054 (2)	0.0001 (16)	−0.0069 (18)	−0.0056 (18)
C13	0.054 (3)	0.049 (2)	0.060 (3)	0.0042 (18)	−0.004 (2)	−0.001 (2)
C14	0.082 (3)	0.051 (3)	0.070 (3)	0.013 (2)	−0.021 (3)	0.005 (2)
C15	0.060 (3)	0.055 (3)	0.095 (4)	0.020 (2)	−0.023 (3)	−0.028 (3)
C16	0.053 (3)	0.075 (3)	0.081 (3)	0.006 (2)	0.001 (3)	−0.021 (3)
C17	0.062 (3)	0.057 (3)	0.066 (3)	−0.005 (2)	−0.002 (2)	−0.001 (2)

Geometric parameters (Å, º)

O1—C6	1.341 (5)	C12—C13	1.378 (6)
O2—C8	1.370 (5)	C13—C14	1.387 (6)
O2—C11	1.438 (5)	C14—C15	1.371 (8)
N1—C3	1.414 (5)	C15—C16	1.374 (8)
N1—C4	1.278 (6)	C16—C17	1.381 (7)
O1—H1O	0.8200	C1—H1	0.9300
C1—C1ⁱ	1.380 (6)	C2—H2	0.9300
C1—C2	1.373 (6)	C4—H4	1.05 (4)
C2—C3	1.395 (5)	C7—H7	0.9300
C3—C3ⁱ	1.399 (5)	C9—H9	0.9300
C4—C5	1.454 (5)	C10—H10	0.9300
C5—C10	1.400 (6)	C11—H11A	0.9700
C5—C6	1.394 (5)	C11—H11B	0.9700
C6—C7	1.403 (5)	C13—H13	0.9300
C7—C8	1.383 (6)	C14—H14	0.9300
C8—C9	1.388 (6)	C15—H15	0.9300
C9—C10	1.371 (6)	C16—H16	0.9300
C11—C12	1.499 (6)	C17—H17	0.9300
C12—C17	1.383 (6)		
C8—O2—C11	117.4 (3)	C12—C17—C16	120.5 (5)
C3—N1—C4	118.9 (4)	C2—C1—H1	120.00
C6—O1—H1O	109.00	C1ⁱ—C1—H1	120.00
C1ⁱ—C1—C2	119.8 (4)	C1—C2—H2	119.00
C1—C2—C3	121.3 (4)	C3—C2—H2	119.00
N1—C3—C3ⁱ	118.3 (3)	N1—C4—H4	122 (2)
C2—C3—C3ⁱ	118.9 (4)	C5—C4—H4	116 (2)

N1—C3—C2	122.8 (4)	C6—C7—H7	120.00
N1—C4—C5	122.2 (4)	C8—C7—H7	120.00
C4—C5—C10	120.5 (4)	C8—C9—H9	120.00
C6—C5—C10	117.7 (3)	C10—C9—H9	120.00
C4—C5—C6	121.8 (4)	C5—C10—H10	119.00
O1—C6—C7	117.5 (3)	C9—C10—H10	119.00
C5—C6—C7	120.7 (4)	O2—C11—H11A	110.00
O1—C6—C5	121.8 (3)	O2—C11—H11B	110.00
C6—C7—C8	119.6 (4)	C12—C11—H11A	110.00
O2—C8—C9	115.0 (4)	C12—C11—H11B	110.00
C7—C8—C9	120.5 (4)	H11A—C11—H11B	108.00
O2—C8—C7	124.5 (3)	C12—C13—H13	120.00
C8—C9—C10	119.2 (4)	C14—C13—H13	120.00
C5—C10—C9	122.3 (4)	C13—C14—H14	120.00
O2—C11—C12	108.6 (3)	C15—C14—H14	120.00
C11—C12—C13	120.9 (4)	C14—C15—H15	120.00
C13—C12—C17	118.8 (4)	C16—C15—H15	120.00
C11—C12—C17	120.3 (4)	C15—C16—H16	120.00
C12—C13—C14	120.8 (4)	C17—C16—H16	120.00
C13—C14—C15	119.8 (4)	C12—C17—H17	120.00
C14—C15—C16	120.0 (5)	C16—C17—H17	120.00
C15—C16—C17	120.2 (5)		
C11—O2—C8—C7	1.5 (6)	C4—C5—C10—C9	179.6 (4)
C11—O2—C8—C9	−177.8 (4)	C6—C5—C10—C9	0.9 (6)
C8—O2—C11—C12	174.0 (3)	O1—C6—C7—C8	177.9 (4)
C4—N1—C3—C2	41.3 (6)	C5—C6—C7—C8	−1.4 (6)
C4—N1—C3—C3^i	−139.8 (4)	C6—C7—C8—O2	−178.4 (4)
C3—N1—C4—C5	−176.8 (4)	C6—C7—C8—C9	0.9 (6)
C1^i—C1—C2—C3	0.1 (8)	O2—C8—C9—C10	179.9 (4)
C2—C1—C1^i—C2^i	0.0 (9)	C7—C8—C9—C10	0.5 (7)
C1—C2—C3—N1	178.9 (5)	C8—C9—C10—C5	−1.4 (7)
C1—C2—C3—C3^i	−0.1 (7)	O2—C11—C12—C13	96.8 (4)
N1—C3—C3^i—N1^i	0.0 (6)	O2—C11—C12—C17	−84.8 (5)
N1—C3—C3^i—C2^i	−179.0 (4)	C11—C12—C13—C14	176.4 (4)
C2—C3—C3^i—N1^i	179.0 (4)	C17—C12—C13—C14	−2.0 (6)
C2—C3—C3^i—C2^i	0.0 (6)	C11—C12—C17—C16	−177.4 (4)
N1—C4—C5—C6	−0.9 (7)	C13—C12—C17—C16	1.0 (7)
N1—C4—C5—C10	−179.5 (4)	C12—C13—C14—C15	1.4 (7)
C4—C5—C6—O1	2.6 (6)	C13—C14—C15—C16	0.2 (7)
C4—C5—C6—C7	−178.2 (4)	C14—C15—C16—C17	−1.2 (8)
C10—C5—C6—O1	−178.8 (4)	C15—C16—C17—C12	0.6 (8)
C10—C5—C6—C7	0.5 (6)		

Symmetry code: (i) −*x*, *y*, *z*.

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C5–C10 phenol ring.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1—H1*O*⋯N1	0.82	1.90	2.622 (5)	147
C2—H2⋯*Cg*2[ii]	0.93	2.88	3.499 (5)	125
C13—H13⋯*Cg*2[iii]	0.93	2.60	3.493 (5)	161

Symmetry codes: (ii) *x*, −*y*+1, *z*−1/2; (iii) *x*, −*y*, *z*+1/2.