2732 measured reflections
2356 independent reflections
911 observed reflections
$[I > 3\sigma(I)]$
3 standard reflections
monitored every 250 reflections
intensity decay: <7.5%

Refinement

Refinement on F
$R = 0.064$
$wR = 0.066$
$S = 1.790$
911 reflections
154 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o) + 0.0001(F_o)^2 + 1]$ (Killean & Lawrence, 1969)
$(\Delta/\sigma)_{\max} = 0.29$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
O(1)	−0.2627 (6)	0.1020 (7)	0.4918 (3)	4.2 (1)
O(2)	0.1969 (5)	0.8969 (8)	0.8399 (3)	4.7 (1)
O(3)	0.3361 (6)	1.1269 (8)	0.9315 (3)	5.4 (1)
O(4)	0.1504 (6)	1.4142 (9)	0.9514 (3)	6.1 (2)
N(1)	−0.0036 (6)	0.2215 (8)	0.6213 (3)	3.4 (1)
N(2)	−0.1053 (7)	0.2437 (8)	0.5668 (3)	3.6 (1)
N(3)	−0.1113 (7)	−0.0673 (8)	0.5607 (3)	3.9 (1)
N(4)	0.0014 (6)	0.7131 (8)	0.8131 (3)	3.5 (1)
C(1)	0.0484 (8)	0.359 (1)	0.6519 (4)	3.4 (1)
C(2)	0.1550 (9)	0.327 (1)	0.7120 (4)	4.3 (2)
C(3)	0.0922 (9)	0.424 (1)	0.7711 (4)	4.3 (2)
C(4)	0.0638 (7)	0.622 (1)	0.7580 (3)	3.2 (2)
C(5)	−0.0431 (8)	0.646 (1)	0.6974 (4)	3.7 (2)
C(6)	0.015 (1)	0.556 (1)	0.6368 (4)	4.2 (2)
C(7)	−0.1656 (8)	0.090 (1)	0.5367 (3)	3.3 (2)
C(8)	0.0708 (8)	0.839 (1)	0.8508 (4)	3.5 (2)
C(9)	−0.0147 (9)	0.908 (1)	0.9065 (4)	5.5 (2)

Table 2. *Selected geometric parameters* (Å, °)

O(1)—C(7)	1.218 (8)	C(1)—C(2)	1.516 (9)
O(2)—C(8)	1.231 (8)	C(1)—C(6)	1.513 (9)
N(1)—N(2)	1.391 (7)	C(2)—C(3)	1.54 (1)
N(1)—C(1)	1.264 (8)	C(3)—C(4)	1.51 (1)
N(2)—C(7)	1.383 (8)	C(4)—C(5)	1.517 (9)
N(3)—C(7)	1.339 (8)	C(5)—C(6)	1.53 (1)
N(4)—C(4)	1.454 (8)	C(8)—C(9)	1.51 (1)
N(4)—C(8)	1.332 (9)		
N(2)—N(1)—C(1)	119.7 (5)	C(3)—C(4)—C(5)	110.5 (5)
N(1)—N(2)—C(7)	117.9 (5)	C(4)—C(5)—C(6)	112.6 (6)
C(4)—N(4)—C(8)	126.0 (6)	C(1)—C(6)—C(5)	109.3 (5)
N(1)—C(1)—C(2)	117.2 (6)	O(1)—C(7)—N(2)	120.5 (6)
N(1)—C(1)—C(6)	128.1 (6)	O(1)—C(7)—N(3)	123.9 (6)
C(2)—C(1)—C(6)	114.8 (6)	N(2)—C(7)—N(3)	115.6 (5)
C(1)—C(2)—C(3)	108.9 (6)	O(2)—C(8)—N(4)	122.0 (6)
C(2)—C(3)—C(4)	112.2 (5)	O(2)—C(8)—C(9)	121.9 (6)
N(4)—C(4)—C(3)	112.5 (5)	N(4)—C(8)—C(9)	116.1 (7)
N(4)—C(4)—C(5)	109.1 (5)		

Intensities were corrected for Lorentz and polarization effects. The structure was solved by direct methods using *MITHRIL* (Gilmore, 1984). H atoms were located by difference Fourier synthesis. Full-matrix least-squares refinement was carried out using the *SDP* package (Enraf–Nonius, 1985). Non-H atoms were refined with isotropic displacement factors, then with anisotropic displacement factors. The isotropic displacement factors for H atoms were arbitrarily assigned as $1.3B_{eq}$ of the attached atoms and not refined. The calculations were performed on a VAX11/785 computer.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, intermolecular distances and least-squares-planes data have been deposited with the IUCr (Reference: CR1118). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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4-(4-Hydroxy-3,5-dimethylphenylazo)benzenesulfonic Acid

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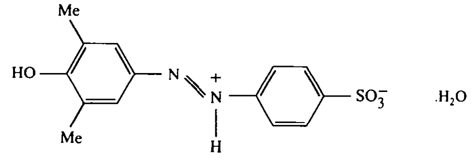
Abstract

In the solid state, the title compound, $C_{14}H_{14}N_2O_4S.H_2O$, exists as two forms: cubes (I) and needles (II). Both kinds of crystal are monohydrates. The dye molecules have the same geometry and are bonded by O—H···O intermolecular hydrogen bonds in both forms: an N^+—H···O^- intermolecular hydrogen bond in (II) and an N^+—H···$(O)_2^-$ bifurcated hydrogen bond in (I).

Comment

There have been many studies on the synthesis and ion-binding properties of chromogenic calixarenes having azo groups (Shinkai, Araki, Shibata, Tsugawa & Manabe, 1989; Nomura, Taniguchi & Tamura, 1989; Nomura, Taniguchi & Otsuji, 1993; Xu & Swagen, 1993; Yeh, Tang, Chen, Liu & Lin, 1994). We are particularly interested in the conformation of azocalixarenes in the solid state and in their interactions with other organic substances (Ehlinger, Lecocq, Perrin & Perrin, 1993). The properties of these azocalixarenes are often compared with those of their non-cyclic analogues (Shinkai *et al.*, 1989; Nomura, Taniguchi & Tamura, 1989; Nomura, Taniguchi & Otsuji, 1993). It is for this purpose that we describe here the crystal structure of 4-(3,5-dimethyl-4-hydroxyphenylazo)benzenesulfonic acid. The crystallization of this product gives two kinds of crystals of the monohydrate: cubes (I) and needles (II).



(I), (II)

In each crystal structure the asymmetric unit contains one dye molecule and one water molecule. The bond lengths are approximately the same in both structures. The N(1)—N(2), C(4)—N(1) and N(2)—C(9) bond lengths indicate that the compound exists as the azo tautomer. The S—O distances are almost equal and have values similar to those found for methylorange (Hanson, 1973). The dihedral angles between the phenyl rings are 11.2 (1) for (I) and 8.9 (1)° for (II), giving almost planar molecules. The difference between the two forms can be explained by the position of the water molecule relative to the C—N=N—C— moiety, as can be seen in Figs. 1 and 2.

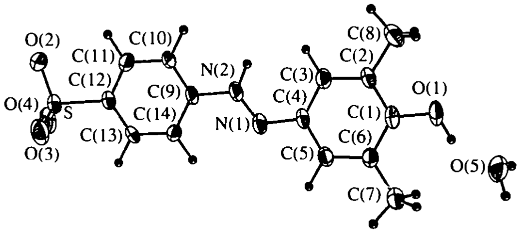


Fig. 1. View of the asymmetric unit of (I) showing the atom-numbering scheme. For non-H atoms, 50% probability ellipsoids are shown.

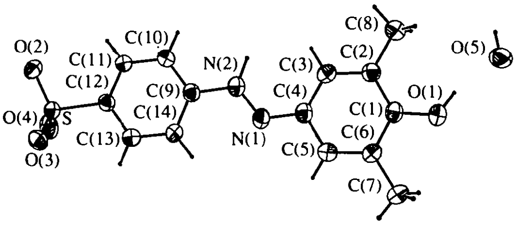


Fig. 2. View of the asymmetric unit of (II) showing the atom-numbering scheme. For non-H atoms, 50% probability ellipsoids are shown.

In (I), intermolecular hydrogen bonds have been found between the water molecule and O(2) and O(4) of two sulfonic groups, and O(1) of the hydroxy group. There is also a bifurcated hydrogen bond between N(2) and two O atoms [O(2) and O(4)] of two sulfonic groups, an H atom being located at 0.959 Å from N(2). This interaction corresponds to a charge-transfer interaction because a proton was transferred from the sulfonic group to N(2) of the azo group.

In (II), intermolecular hydrogen bonds have been found between the water molecule and O(3) and O(4) of two sulfonic groups, and O(1) of the hydroxyl group. We also find a fourth interaction between N(2) and O(2) which corresponds to a charge-transfer interaction, the H atom being located at 0.945 Å from N(2).

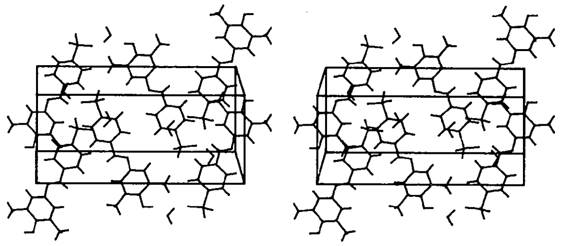


Fig. 3. Packing along [100] for (I).

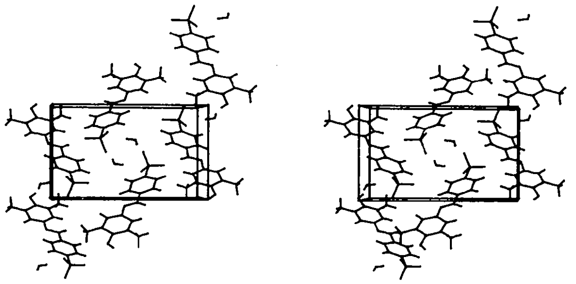


Fig. 4. Packing along [100] for (II).

Experimental

The title compound was prepared by a diazo coupling reaction of 2,6-dimethylphenol and diazoted sodium sulfanilate in water at *ca* 275 K. At the end of the reaction, the red solution was treated with hydrochloric acid and *p*-(4-hydroxy-3,5-dimethylphenylazo)benzenesulfonic acid was isolated by filtration and recrystallized from water (63% yield). ^{1}H NMR (D_2O): δ 2.18 (6H, *s*, CH_3), 7.43 (2H, *s*, ArH in the phenol moiety), 7.70 and 7.87 p.p.m. (both 2H, *d*, ArH in the 4-sulfonic phenyl moiety). Elemental analysis: calculated for $C_{14}H_{14}N_2O_4S.H_2O$, C 51.84, H 4.97, N 8.64, S 9.88%; found, C 51.70, H 4.91, N 8.66, S 9.89%.

Form (I)

Crystal data

$C_{14}H_{14}N_2O_4S.H_2O$
$M_r = 324.35$
Monoclinic
$P2_1/n$
$a = 9.636$ (2) Å
$b = 19.634$ (3) Å
$c = 8.215$ (2) Å
$\beta = 107.45$ (2)°

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 25 reflections
$\theta = 8$–52°
$\mu = 2.135$ mm^{-1}
$T = 295$ K
Cube

$V = 1482$ (1) Å^3
$Z = 4$
$D_x = 1.453$ Mg m^{-3}

0.6 × 0.6 × 0.6 mm
Red

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction:
  ψ scan
  $T_{\min} = 0.807$, $T_{\max} = 0.997$
6470 measured reflections
2953 independent reflections

1226 observed reflections
  $[I > 2\sigma(I)]$
$R_{\rm int} = 0.0486$
$\theta_{\max} = 73°$
$h = 0 \rightarrow 11$
$k = -24 \rightarrow 24$
$l = -10 \rightarrow 10$
3 standard reflections
  frequency: 60 min
  intensity decay: 7.7%

Refinement

Refinement on F^2
$R(F) = 0.0486$
$wR(F^2) = 0.1098$
$S = 0.886$
2953 reflections
213 parameters
Only coordinates of H atoms refined
$w = 1/\{\sigma^2(F_o^2) + [0.0112(F_o^2 + 2F_c^2)]^2\}$

$(\Delta/\sigma)_{\max} = -0.196$
$\Delta\rho_{\max} = 0.21$ e Å^{-3}
$\Delta\rho_{\min} = -0.47$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C)

Form (II)

Crystal data

$C_{14}H_{14}N_2O_4S.H_2O$
$M_r = 324.35$
Monoclinic
$P2_1/n$
$a = 14.586$ (2) Å
$b = 8.583$ (1) Å
$c = 12.186$ (2) Å
$\beta = 101.83$ (2)°
$V = 1493$ (1) Å^3
$Z = 4$
$D_x = 1.443$ Mg m^{-3}

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 25 reflections
$\theta = 15$–$51°$
$\mu = 2.120$ mm^{-1}
$T = 295$ K
Needle
1.0 × 0.3 × 0.3 mm
Red

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction:
  ψ scan
  $T_{\min} = 0.723$, $T_{\max} = 0.996$
6239 measured reflections
2972 independent reflections

2106 observed reflections
  $[I > 2\sigma(I)]$
$R_{\rm int} = 0.0393$
$\theta_{\max} = 73°$
$h = -18 \rightarrow 18$
$k = -10 \rightarrow 10$
$l = 0 \rightarrow 15$
3 standard reflections
  frequency: 60 min
  intensity decay: 6.5%

Refinement

Refinement on F^2
$R(F) = 0.0393$
$wR(F^2) = 0.1077$
$S = 0.994$
2972 reflections
216 parameters
Only coordinates of H atoms refined

$w = 1/\{\sigma(F_o^2) + [0.0225(F_o^2 + 2F_c^2)]^2\}$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.57$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (I)

$$B_{\rm eq} = (8\pi^2/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
O(1)	0.4059 (3)	−0.0166 (1)	−0.8028 (3)	3.53 (7)
C(1)	0.3371 (4)	−0.0007 (2)	−0.6905 (4)	2.63 (9)
C(2)	0.2872 (4)	0.0671 (2)	−0.6990 (4)	2.45 (9)
C(3)	0.2125 (4)	0.0884 (2)	−0.5890 (4)	2.71 (9)
C(4)	0.1912 (4)	0.0419 (2)	−0.4671 (4)	2.40 (8)
C(5)	0.2417 (4)	−0.0247 (2)	−0.4605 (4)	2.56 (9)
C(6)	0.3132 (4)	−0.0485 (2)	−0.5710 (4)	2.45 (9)
C(7)	0.3637 (4)	−0.1206 (2)	−0.5671 (4)	3.4 (1)
C(8)	0.3159 (4)	0.1147 (2)	−0.8299 (5)	3.5 (1)
N(1)	0.1240 (3)	0.0570 (1)	−0.3456 (3)	2.58 (8)
N(2)	0.0792 (3)	0.1174 (2)	−0.3361 (4)	2.87 (9)
C(9)	0.0131 (4)	0.1367 (2)	−0.2098 (4)	2.26 (9)
C(10)	−0.0124 (4)	0.2046 (2)	−0.1942 (4)	2.9 (1)
C(11)	−0.0727 (4)	0.2262 (2)	−0.0694 (4)	3.0 (1)
C(12)	−0.1074 (4)	0.1784 (2)	0.0378 (4)	2.35 (9)
C(13)	−0.0838 (4)	0.1101 (2)	0.0177 (4)	2.7 (1)
C(14)	−0.0236 (4)	0.0879 (2)	−0.1062 (4)	2.55 (9)
S	−0.1782 (1)	0.20632 (5)	0.2028 (1)	2.79 (2)
O(2)	−0.2072 (3)	0.2783 (1)	0.1729 (3)	3.47 (7)
O(3)	−0.0668 (3)	0.1928 (2)	0.3606 (3)	4.59 (8)
O(4)	−0.3090 (3)	0.1663 (1)	0.1832 (3)	4.02 (8)
O(5)	0.5056 (4)	−0.1289 (2)	−0.8734 (4)	4.9 (1)

Table 2. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (II)

$$B_{\rm eq} = (8\pi^2/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
O(1)	−0.1332 (1)	0.9763 (2)	1.1363 (1)	3.58 (4)
C(1)	−0.0975 (1)	0.8795 (2)	1.0729 (2)	2.66 (4)
C(2)	−0.0007 (1)	0.8393 (2)	1.0933 (2)	2.54 (4)
C(3)	0.0295 (1)	0.7420 (2)	1.0194 (2)	2.63 (4)
C(4)	−0.0337 (1)	0.6800 (2)	0.9260 (2)	2.71 (4)
C(5)	−0.1297 (1)	0.7168 (3)	0.9105 (2)	3.24 (5)
C(6)	−0.1630 (1)	0.8164 (2)	0.9805 (2)	3.10 (4)
C(7)	−0.2643 (2)	0.8627 (3)	0.9627 (2)	4.65 (6)
C(8)	0.0664 (2)	0.9028 (3)	1.1931 (2)	3.58 (5)
N(1)	−0.0124 (1)	0.5857 (2)	0.8451 (1)	2.81 (4)
N(2)	0.0725 (1)	0.5473 (2)	0.8468 (1)	2.67 (4)
C(9)	0.0933 (1)	0.4532 (2)	0.7596 (2)	2.44 (4)
C(10)	0.1829 (1)	0.3938 (2)	0.7729 (2)	2.82 (4)
C(11)	0.2059 (1)	0.3018 (2)	0.6891 (2)	2.72 (4)
C(12)	0.1387 (1)	0.2684 (2)	0.5938 (2)	2.37 (4)
C(13)	0.0491 (1)	0.3297 (3)	0.5819 (2)	3.39 (5)
C(14)	0.0254 (1)	0.4224 (3)	0.6645 (2)	3.29 (5)
S	0.16530 (3)	0.14628 (6)	0.48728 (4)	2.51 (1)
O(2)	0.26688 (9)	0.1426 (2)	0.5038 (1)	3.50 (3)
O(3)	0.1212 (1)	0.2173 (2)	0.3820 (1)	3.45 (3)
O(4)	0.1258 (1)	−0.0050 (2)	0.5044 (1)	3.85 (4)
O(5)	−0.0647 (1)	1.1321 (2)	1.3127 (1)	3.74 (4)

Table 3. *Selected geometric parameters* (Å, °) *for* (I)

O(1)—C(1)	1.324 (5)	C(1)—C(2)	1.410 (5)
C(2)—C(3)	1.378 (5)	C(3)—C(4)	1.415 (5)
C(4)—C(5)	1.389 (5)	C(5)—C(6)	1.376 (5)
C(6)—C(7)	1.494 (5)	C(1)—C(6)	1.425 (5)
C(2)—C(8)	1.511 (5)	C(4)—N(1)	1.375 (5)
N(1)—N(2)	1.272 (4)	N(2)—C(9)	1.421 (5)
C(9)—C(10)	1.370 (5)	C(10)—C(11)	1.387 (6)
C(11)—C(12)	1.394 (5)	C(12)—C(13)	1.379 (5)
C(13)—C(14)	1.385 (5)	C(9)—C(14)	1.395 (5)
C(12)—S	1.777 (4)	S—O(2)	1.448 (3)
S—O(3)	1.438 (2)	S—O(4)	1.453 (3)

O(1)—C(1)—C(2)	114.9 (3)	C(1)—C(6)—C(5)	116.6 (3)
O(1)—C(1)—C(6)	122.9 (3)	C(1)—C(6)—C(7)	121.3 (3)
C(2)—C(1)—C(6)	122.1 (4)	C(5)—C(6)—C(7)	122.1 (3)
C(1)—C(2)—C(3)	119.4 (3)	C(4)—N(1)—N(2)	119.2 (3)
C(1)—C(2)—C(8)	119.1 (3)	N(1)—N(2)—C(9)	121.9 (3)
C(3)—C(2)—C(8)	121.5 (3)	N(2)—C(9)—C(10)	117.4 (3)
C(2)—C(3)—C(4)	118.9 (3)	N(2)—C(9)—C(14)	120.9 (3)
C(3)—C(4)—C(5)	120.7 (3)	C(10)—C(9)—C(14)	121.7 (4)
C(3)—C(4)—N(1)	125.0 (3)	C(9)—C(10)—C(11)	119.6 (3)
C(5)—C(4)—N(1)	114.2 (3)	C(10)—C(11)—C(12)	119.6 (3)
C(4)—C(5)—C(6)	122.2 (3)	C(11)—C(12)—C(13)	120.0 (4)
C(11)—C(12)—S	119.6 (3)	C(9)—C(14)—C(13)	118.1 (3)
C(13)—C(12)—S	120.4 (3)	C(12)—C(13)—C(14)	121.0 (3)
C(12)—S—O(2)	105.7 (2)	C(12)—S—O(3)	106.1 (2)
C(12)—S—O(4)	105.5 (2)	O(2)—S—O(3)	112.8 (2)
O(2)—S—O(4)	113.1 (2)	O(3)—S—O(4)	112.9 (2)

C(5)—C(4)—N(1)—N(2)	177.1 (3)
C(4)—N(1)—N(2)—C(9)	−177.9 (3)
N(1)—N(2)—C(9)—C(10)	170.8 (3)

D—H···*A*	*D*···*A*	*D*—H···*A*
O(1)—H(1)···O(5)	2.541 (4)	151 (3)
N(2)—H(20)···O(2^{i})	2.889 (4)	124 (3)
N(2)—H(20)···O(3^{ii})	2.877 (4)	124 (3)
O(5)—H(50)···O(2^{iii})	2.809 (4)	173 (4)
O(5)—H(51)···O(4^{iv})	2.778 (4)	161 (4)

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

Table 4. *Selected geometric parameters* (Å, °) *for* (II)

O(1)—C(1)	1.313 (3)	C(1)—C(2)	1.424 (3)
C(2)—C(3)	1.365 (3)	C(3)—C(4)	1.413 (2)
C(4)—C(5)	1.411 (3)	C(5)—C(6)	1.366 (3)
C(6)—C(7)	1.501 (3)	C(1)—C(6)	1.426 (3)
C(2)—C(8)	1.499 (3)	C(4)—N(1)	1.359 (3)
N(1)—N(2)	1.276 (2)	N(2)—C(9)	1.417 (3)
C(9)—C(10)	1.380 (3)	C(10)—C(11)	1.386 (3)
C(11)—C(12)	1.386 (2)	C(12)—C(13)	1.388 (3)
C(13)—C(14)	1.382 (3)	C(9)—C(14)	1.386 (3)
C(12)—S	1.773 (2)	S—O(2)	1.454 (1)
S—O(3)	1.447 (1)	S—O(4)	1.453 (2)
O(1)—C(1)—C(2)	123.3 (2)	C(1)—C(6)—C(5)	117.6 (2)
O(1)—C(1)—C(6)	115.0 (2)	C(1)—C(6)—C(7)	119.6 (2)
C(2)—C(1)—C(6)	121.7 (2)	C(5)—C(6)—C(7)	122.8 (2)
C(1)—C(2)—C(3)	118.4 (2)	C(4)—N(1)—N(2)	120.4 (2)
C(1)—C(2)—C(8)	120.8 (2)	N(1)—N(2)—C(9)	119.4 (2)
C(3)—C(2)—C(8)	120.8 (2)	N(2)—C(9)—C(10)	117.8 (2)
C(2)—C(3)—C(4)	121.1 (2)	N(2)—C(9)—C(14)	120.6 (2)
C(3)—C(4)—C(5)	119.2 (2)	C(10)—C(9)—C(14)	121.6 (2)
C(3)—C(4)—N(1)	126.9 (2)	C(9)—C(10)—C(11)	119.3 (2)
C(5)—C(4)—N(1)	113.9 (2)	C(10)—C(11)—C(12)	119.9 (2)
C(4)—C(5)—C(6)	121.8 (2)	C(11)—C(12)—C(13)	119.9 (2)
C(9)—C(14)—C(13)	118.4 (2)	C(11)—C(12)—S	120.8 (1)
C(13)—C(12)—S	119.3 (1)	C(12)—C(13)—C(14)	120.8 (2)
C(12)—S—O(2)	106.33 (8)	C(12)—S—O(3)	106.05 (9)
C(12)—S—O(4)	105.7 (1)	O(2)—S—O(3)	112.76 (9)
O(2)—S—O(4)	112.56 (9)	O(3)—S—O(4)	112.76 (9)

C(5)—C(4)—N(1)—N(2)	177.7 (3)
C(4)—N(1)—N(2)—C(9)	−177.9 (3)
N(1)—N(2)—C(9)—C10)	−170.0 (3)

D—H···*A*	*D*···*A*	*D*—H···*A*
O(1)—H(1)···O(5)	2.555 (4)	163 (3)
N(2)—H(20)···O(2^{i})	2.779 (3)	167 (3)
O(5)—H(50)···O(4^{ii})	2.787 (5)	168 (3)
O(5)—H(51)···O(3^{iii})	2.768 (2)	168 (3)

Symmetry codes: (i) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z$; (ii) $-x, 1-y, 2-z$; (iii) $x, 1+y, 1+z$.

In both structures, H atoms bonded to C atoms were placed in calculated positions. H atoms bonded to N atoms and O atoms were located in difference maps.

Data reduction: *SDP* (B. A. Frenz & Associates Inc., 1982). Program(s) used to solve structures: *MULTAN*80 (Main *et al.*, 1980). Program(s) used to refine structures: *SHELXL*93 (Sheldrick, 1993). Program used for geometric calculations: *PARST* (Nardelli, 1983).

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: PA1174). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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(2-Methoxyphenyl)(phenyl)vinylphosphine Oxide

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Abstract

In the molecule of the title compound, $C_{15}H_{15}O_2P$, the C═C—P═O fragment has an *S-cis* conformation. The methoxyphenyl ring assumes an almost coplanar arrangement with the P═O bond and is almost perpendicular to the phenyl ring.