

S. Thamocharan,<sup>a</sup>  
V. Parthasarathi,<sup>a\*</sup> S. M. Anitha,<sup>a</sup>  
Archana Prasad,<sup>b</sup> T. R. Rao<sup>b</sup> and  
Anthony Linden<sup>c</sup><sup>a</sup>Department of Physics, Bharathidasan  
University, Tiruchirappalli 620 024, India,<sup>b</sup>Department of Chemistry, Banaras Hindu  
University, Varanasi 221 005, India, and<sup>c</sup>Institute of Organic Chemistry, University of  
Zürich, Winterthurerstrasse 190, CH-8057  
Zürich, Switzerland

Correspondence e-mail: vpsarati@yahoo.com

## Key indicators

Single-crystal X-ray study

T = 160 K

Mean  $\sigma(C-C)$  = 0.003 Å

R factor = 0.043

wR factor = 0.112

Data-to-parameter ratio = 10.8

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

## N-(4-Butylphenyl)salicylalimine at 160 K

In the title compound, C<sub>17</sub>H<sub>19</sub>NO, which is a Schiff base, an intramolecular O—H···N hydrogen bond involving the hydroxy group forms a six-membered ring with a graph-set motif of *S*(6). Several intermolecular C—H··· $\pi$  interactions occur between adjacent molecules which are arranged perpendicular to one another.

## Comment

Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964; Hadjoudis *et al.*, 1987). It is known that molecules exhibiting photochromism are non-planar (Moustakali-Mavridis *et al.*, 1978). In view of this, an X-ray crystal structure determination of the title compound, (I), has been carried out to investigate the planarity of the molecule in the solid state.

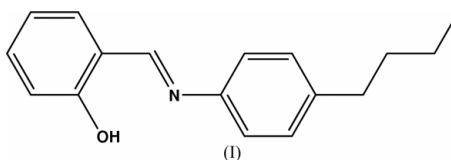


Fig. 1 shows the asymmetric unit of (I) with the atomic numbering scheme. The corresponding bond lengths and angles in (I) are comparable with those in the related structures, *N*-salicylidene-2-aminopyridine, 3-methyl-*N*-(3-methoxysalicylidene)-2-aminopyridine, *N*-(5-bromosalicylidene)-2-aminopyridine and 5-chloro-*N*-(5-methoxysalicylidene)-2-aminopyridine (Moustakali-Mavridis *et al.*, 1978), *N*-(5-chlorosalicylidene)-2-hydroxy-5-chloroaniline (Elerman *et al.*, 2002) and *N*-(2-fluoro-3-methoxy)salicylidene (Ünver *et al.*, 2002). The butyl group projects in a planar zigzag fashion directly away from and perpendicular to the central aromatic ring plane [ $C13-C12-C15-C16 = 88.4(2)^\circ$ ]. The dihedral angle between the planes of the two aromatic rings is  $11.46(10)^\circ$ , which shows that the conjugated part of the molecule is not entirely planar.

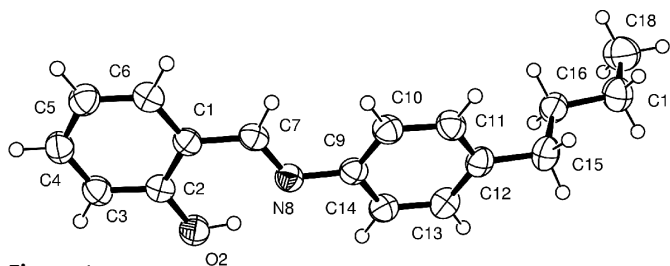


Figure 1

View of the asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary radii.

Received 20 October 2003

Accepted 22 October 2003

Online 31 October 2003

In the crystal structure, the hydroxy group forms an intramolecular hydrogen bond with the N atom, thereby completing a six-membered ring which has a graph-set motif of  $S(6)$  (Bernstein *et al.*, 1995). Atom C11 (*via* H11) in the butyl-substituted phenyl ring acts as a donor for a weak intermolecular C—H $\cdots\pi$  interaction with the hydroxy-substituted phenyl ring (centroid Cg1) in the molecule at  $(2 - x, \frac{1}{2} + y, \frac{3}{2} - z)$ . Atom C14 (*via* H14), which is *para* to C11, is involved in a weak intermolecular C—H $\cdots\pi$  interaction with the hydroxy-substituted phenyl ring of another molecule lying in the opposite direction at  $(1 - x, y - \frac{1}{2}, \frac{3}{2} - z)$ . Atoms C3 (*via* H3) and C6 (*via* H6), which lie *para* with respect to each other in the hydroxy-substituted phenyl ring, are also involved in weak intermolecular C—H $\cdots\pi$  interactions with the butyl-substituted phenyl ring (centroid Cg2) in the molecules at  $(1 - x, y - \frac{1}{2}, \frac{3}{2} - z)$  and  $(2 - x, \frac{1}{2} + y, \frac{3}{2} - z)$ , respectively (Table 1). These interactions result from the adjacent molecules being stacked perpendicular to one another along the [110] direction.

## Experimental

The title Schiff base was synthesized by refluxing absolute ethanol solutions of salicylaldehyde (15 mmol) and 4-butaniline (15 mmol) for 2 h and leaving the solution overnight. The product was filtered off by suction, thoroughly washed with cold ethanol and recrystallized from absolute ethanol (yield 70%; m.p. 311–338 K).

### Crystal data

C<sub>17</sub>H<sub>19</sub>NO  
*M<sub>r</sub>* = 253.33  
 Orthorhombic,  $P2_12_12_1$   
*a* = 5.5848 (1) Å  
*b* = 8.0987 (2) Å  
*c* = 31.2943 (6) Å  
*V* = 1415.43 (5) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.189 Mg m<sup>-3</sup>

Mo *K*α radiation  
 Cell parameters from 1931 reflections  
 $\theta$  = 2.0–27.5°  
 $\mu$  = 0.07 mm<sup>-1</sup>  
*T* = 160 (2) K  
 Prism, colourless  
 0.25 × 0.23 × 0.18 mm

### Data collection

Nonius KappaCCD diffractometer  
 $\varphi$  and  $\omega$  scans with  $\kappa$  offsets  
 18 762 measured reflections  
 1917 independent reflections  
 1474 reflections with  $I > 2\sigma(I)$

$R_{\text{int}}$  = 0.058  
 $\theta_{\text{max}}$  = 27.5°  
 $h = -7 \rightarrow 7$   
 $k = -8 \rightarrow 10$   
 $l = -40 \rightarrow 40$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.112$   
*S* = 1.03  
 1917 reflections  
 177 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0691P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.16 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.13 \text{ e } \text{Å}^{-3}$

**Table 1**

Hydrogen-bonding geometry (Å, °).

Cg1 is the centroid of ring C1–C6 and Cg2 is the centroid of ring C9–C14.

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O2—H2 $\cdots$ N8	0.90 (2)	1.81 (2)	2.598 (2)	144 (2)
C11—H11 $\cdots$ Cg1 <sup>i</sup>	0.95	3.10	3.7998 (19)	132
C14—H14 $\cdots$ Cg1 <sup>ii</sup>	0.95	2.97	3.7003 (18)	135
C3—H3 $\cdots$ Cg2 <sup>ii</sup>	0.95	2.98	3.7585 (19)	140
C6—H6 $\cdots$ Cg2 <sup>i</sup>	0.95	2.81	3.5976 (19)	141

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

The position of the hydroxy H atom was determined from a difference Fourier map and refined along with its isotropic displacement parameter, while restraining the O—H bond length to 0.82 (2) Å. The methyl H atoms were constrained to an ideal geometry (C—H = 0.98 Å), with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ , but were allowed to rotate freely about the C—C bonds. All the remaining H atoms were placed in geometrically idealized positions (C—H = 0.95–0.99 Å) and constrained to ride on their parent atoms with  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ . Although the molecule is achiral, the crystal structure is chiral. Because of the absence of any significant anomalous scatterers in the compound, attempts to refine the Flack (1983) parameter with 1320 Friedel pairs led to an inconclusive value (Flack & Bernardinelli, 2000) of  $-1.2(16)$ . Therefore, the absolute structure was assigned arbitrarily and the Friedel pairs were merged before the final refinement.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

## References

- Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.  
 Bernstein, J., Davis, R. E., Shimon, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.  
 Cohen, M. D., Schmidt, G. M. J. & Flavian, S. (1964). *J. Chem. Soc.* pp. 2041–2051.  
 Elerman, Y., Kabak, M. & Eimali, A. (2002). *Z. Naturforsch. Teil B*, **57**, 651–656.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
 Flack, H. D. & Bernardinelli, G. (2000). *J. Appl. Cryst.* **33**, 1143–1148.  
 Hadjoudis, E., Vittorakis, M. & Moustakali-Mavridis, I. (1987). *Tetrahedron*, **43**, 1345–1360.  
 Moustakali-Mavridis, I., Hadjoudis, E. & Mavridis, A. (1978). *Acta Cryst.* **B34**, 3709–3715.  
 Nonius (2000). *COLLECT*. Nonius BV, Delft, The Netherlands.  
 Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.  
 Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.  
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.  
 Ünver, H., Kendi, E., Güven, K. & Durlu, T. N. (2002). *Z. Naturforsch. Teil B*, **57**, 685–690.