

LEHMANN, M. S. & LARSEN, F. K. (1974). *Acta Cryst.* **A30**, 580–589.  
 RIZZOLI, C., SANGERMANO, V., CALESTANI, G. & ANDRETTI, G. D. (1987). *J. Appl. Cryst.* **20**, 436–439.

SHELDRIK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.  
 UGOZZOLI, F. (1987). *Comput. Chem.* **11**(2), 109–120.  
 WALKER, N. & STUART, D. (1983). *Acta Cryst.* **A39**, 158–166.

*Acta Cryst.* (1990). **C46**, 2259–2260

## Stereochemical Studies of Oligomers. XXVIII.\* 4,4'-Bis(*p*-aminophenoxy)diphenyl Sulfone

BY GABRIELE BOCELLI

*Centro di Studio per la Strutturistica Diffraattometrica del CNR, Viale delle Scienze, 43100 Parma, Italy*

AND CORRADO RIZZOLI

*Istituto di Strutturistica Chimica, Università di Parma, Viale delle Scienze, 43100 Parma, Italy*

(Received 25 January 1990; accepted 19 April 1990)

**Abstract.**  $C_{27}H_{20}N_2O_4$ ,  $M_r = 436.47$ , monoclinic,  $P2_1/c$ ,  $a = 21.442$  (3),  $b = 9.954$  (2),  $c = 9.934$  (2) Å,  $\beta = 94.69$  (4)°,  $V = 2113.2$  Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.37$  g cm<sup>-3</sup>,  $\lambda(\text{Cu } K\alpha) = 1.5418$  Å,  $\mu = 7.17$  cm<sup>-1</sup>,  $F(000) = 912$ , room temperature, final  $R = 0.057$  for 3308 reflections with  $I \geq 2\sigma(I)$ . The molecule adopts a butterfly conformation with the C—S—C angle [107.6 (2)°] comparable with that [106.1 (1)°] observed in 4,4'-diaminodiphenyl sulfone [Bocelli & Cantoni (1990). *Acta Cryst.* **C46**, 2257–2259]. The dihedral angles between the individual planar rings  $A-B$ ,  $A-C$ ,  $A-D$ ,  $B-C$ ,  $B-D$  and  $C-D$  are 98.3 (1), 28.0 (1), 50.9 (1), 70.7 (1), 42.5 (1) and 77.3 (1)°, respectively. Intermolecular contacts  $< 2.5$  Å are:  $N1 \cdots H27^i = 2.48$  (4),  $O4 \cdots H20^{ii} = 2.49$  (3) and  $C23 \cdots H1N2^{iii} = 2.40$  (3) Å [(i)  $-x, -y, -z$ ; (ii)  $x, -y - \frac{1}{2}, z + \frac{1}{2}$ ; (iii)  $x, -y + \frac{1}{2}, z + \frac{1}{2}$ ].

**Experimental.** Colorless prismatic crystal approximately  $0.32 \times 0.57 \times 0.67$  mm, diffraction data collected on a Siemens AED single-crystal diffractometer equipped with an IBM PS2/30 personal computer, unit-cell parameters obtained from a least-squares fit to the angular values of 29 reflections ( $11.3 \leq \theta \leq 44.3^\circ$ ) accurately centred on the diffractometer, reflections measured using a modified version (Belletti, Cantoni & Pasquinelli, 1988) of the Lehmann & Larsen (1974) method. One standard reflection monitored every 50 measurements showed no decrease in intensity. Intensities corrected for Lorentz and polarization effects but not for absorption. A total of 4486 reflections collected (index range):  $h -26/26$ ,  $k 0/12$ ,  $l 0/12$  in the  $\theta$  range  $3-70^\circ$ ; 4102 independent ( $R_{int} = 0.015$ ) and 3326 with

$I \geq 2\sigma(I)$  considered observed. Structure solved by direct methods with *SHELX76* (Sheldrick, 1976), anisotropic block-matrix least-squares refinement, H atoms found from a difference Fourier map refined with isotropic temperature factors.  $\sum w\Delta F^2$  minimized, unit weights, 14 reflections omitted because they were probably affected by extinction. The highest peak in the final  $\Delta F$  map was  $0.35$  e Å<sup>-3</sup>, final  $R$

Table 1. Atomic fractional coordinates ( $\times 10^4$ ) and  $U_{eq}$  values (Å<sup>2</sup>  $\times 10^4$ )

	$x$	$y$	$z$	$U_{eq}^*$
S	2504 (1)	668 (1)	2993 (1)	548 (2)
O1	-85 (1)	2162 (2)	1214 (2)	697 (8)
O2	3840 (1)	-1260 (2)	-1571 (2)	667 (7)
O3	2779 (1)	1922 (2)	3436 (2)	758 (8)
O4	2487 (1)	-418 (3)	3946 (2)	709 (8)
N1	-2292 (2)	220 (4)	3075 (4)	790 (13)
N2	5033 (2)	2159 (2)	-4998 (3)	714 (10)
C4	1722 (1)	1011 (3)	2397 (3)	487 (8)
C5	1596 (1)	2070 (3)	1504 (3)	632 (10)
C6	987 (2)	2421 (3)	1133 (3)	649 (11)
C7	499 (1)	1723 (3)	1654 (3)	513 (7)
C8	619 (1)	650 (3)	2521 (3)	518 (8)
C9	1233 (1)	289 (3)	2885 (3)	508 (8)
C10	-613 (1)	1585 (3)	1750 (3)	555 (9)
C11	-772 (1)	1934 (3)	3016 (3)	598 (10)
C12	-1331 (1)	1467 (3)	3464 (3)	603 (10)
C13	-1715 (1)	645 (3)	2647 (3)	573 (9)
C14	-1549 (2)	285 (4)	1407 (3)	680 (11)
C15	-988 (2)	763 (4)	939 (3)	639 (10)
C16	2896 (1)	107 (3)	1616 (3)	477 (7)
C17	3242 (1)	1020 (3)	921 (3)	590 (9)
C18	3558 (1)	589 (3)	-157 (3)	580 (10)
C19	3533 (1)	-739 (3)	-521 (3)	506 (8)
C20	3194 (1)	-1654 (3)	158 (3)	592 (9)
C21	2873 (1)	-1234 (3)	1233 (3)	555 (9)
C22	4150 (1)	-374 (3)	-2403 (3)	539 (9)
C23	4758 (1)	5 (3)	-2063 (3)	570 (9)
C24	5056 (1)	847 (3)	-2926 (3)	559 (8)
C25	4749 (1)	1287 (2)	-4140 (3)	513 (8)
C26	4136 (1)	851 (3)	-4460 (3)	578 (9)
C27	3841 (1)	38 (3)	-3594 (3)	601 (9)

\* Part XXVII: Bocelli & Cantoni (1990).

\* Hamilton (1959).

Table 2. Bond distances (Å) and angles (°)

S—O3	1.434 (2)	C10—C15	1.363 (5)
S—O4	1.439 (3)	C11—C12	1.392 (4)
S—C4	1.765 (3)	C12—C13	1.377 (4)
S—C16	1.754 (3)	C13—C14	1.358 (4)
O1—C7	1.364 (3)	C14—C15	1.408 (6)
O1—C10	1.412 (3)	C16—C17	1.392 (4)
O2—C19	1.379 (4)	C16—C21	1.388 (4)
O2—C22	1.412 (4)	C17—C18	1.382 (4)
N1—C13	1.406 (5)	C18—C19	1.370 (4)
N2—C25	1.391 (4)	C19—C20	1.376 (4)
C4—C5	1.390 (4)	C20—C21	1.382 (4)
C4—C9	1.391 (4)	C22—C23	1.373 (3)
C5—C6	1.373 (5)	C22—C27	1.371 (4)
C6—C7	1.391 (5)	C23—C24	1.391 (4)
C7—C8	1.383 (4)	C24—C25	1.396 (4)
C8—C9	1.384 (3)	C25—C26	1.396 (3)
C10—C11	1.374 (4)	C26—C27	1.373 (4)
C4—S—C16	107.6 (1)	C12—C13—C14	120.2 (3)
O4—S—C16	108.3 (1)	N1—C13—C14	119.8 (3)
O4—S—C4	106.9 (1)	C13—C14—C15	120.3 (3)
O3—S—C16	107.8 (1)	C10—C15—C14	119.1 (2)
O3—S—C4	106.9 (1)	S—C16—C21	120.8 (2)
O3—S—O4	118.9 (1)	S—C16—C17	119.2 (2)
C7—O1—C10	119.5 (2)	C17—C16—C21	120.0 (2)
C19—O2—C22	119.0 (2)	C16—C17—C18	119.8 (2)
S—C4—C9	120.4 (2)	C17—C18—C19	119.5 (2)
S—C4—C5	119.4 (2)	O2—C19—C18	123.5 (2)
C5—C4—C9	120.1 (2)	C18—C19—C20	121.3 (2)
C4—C5—C6	119.7 (2)	O2—C19—C20	115.2 (2)
C5—C6—C7	120.1 (3)	C19—C20—C21	119.7 (2)
O1—C7—C6	114.8 (2)	C16—C21—C20	119.6 (2)
C6—C7—C8	120.7 (2)	O2—C22—C27	118.3 (2)
O1—C7—C8	124.5 (2)	O2—C22—C23	120.7 (2)
C7—C8—C9	119.2 (2)	C23—C22—C27	120.8 (2)
C4—C9—C8	120.2 (2)	C22—C23—C24	119.3 (2)
O1—C10—C15	118.3 (2)	C23—C24—C25	120.9 (2)
O1—C10—C11	120.6 (2)	N2—C25—C24	121.7 (2)
C11—C10—C15	120.9 (3)	C24—C25—C26	117.9 (2)
C10—C11—C12	119.5 (2)	N2—C25—C26	120.4 (2)
C11—C12—C13	119.9 (2)	C25—C26—C27	120.9 (2)
N1—C13—C12	119.9 (2)	C22—C27—C26	120.2 (2)

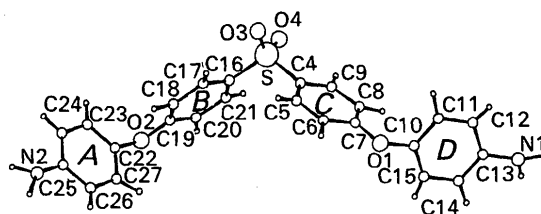


Fig. 1. Projection of the molecule.

Atomic parameters for non-H atoms are given in Table 1;\* Table 2 contains bond distances and angles while the arbitrary labelling of atoms is shown in Fig. 1.

**Related literature.** This structure is one of a series of oligomers related to polymers which are of interest because of their technological properties.

\* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates with their isotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53028 (22 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

#### References

- BELLETTI, D., CANTONI, A. & PASQUINELLI, G. (1988). *Gestione on Line di Diffratometro a Cristallo Singolo Siemens AED con Sistema IBM PS2/30*. Internal Report 1/88. Centro di Studio per la Strutturistica Diffraattometrica del CNR, Parma, Italy.
- BOCELLI, G. & CANTONI, A. (1990). *Acta Cryst.* **C46**, 2257–2259.
- HAMILTON, W. C. (1959). *Acta Cryst.* **12**, 609–610.
- LEHMANN, M. S. & LARSEN, F. K. (1974). *Acta Cryst.* **A30**, 580–589.
- RIZZOLI, C., SANGERMANO, V., CALESTANI, G. & ANDRETTI, G. D. (1987). *J. Appl. Cryst.* **20**, 436–439.
- SHELDRIK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

= 0.057. Atomic scattering factors from *SHELX76*. All calculations performed on an IBM PS2/80 personal computer with the *CRYSRULER* package (Rizzoli, Sangermano, Calestani & Andreotti, 1987).

*Acta Cryst.* (1990). **C46**, 2260–2262

## Structure of 6-(2-Hydroxyphenyl)pyridine-2-carbonitrile

BY KENTARO YAMAGUCHI, YOSHIKUNI ITOH,\* TAKASHI ITOH, AKIO OHSAWA AND HIROSHI IGETA

*School of Pharmaceutical Sciences, Showa University, 1-5-8, Hatanodai, Shinagawa-ku, Tokyo 142, Japan*

(Received 29 March 1990; accepted 1 May 1990)

**Abstract.**  $C_{12}H_8N_2O$ ,  $M_r = 196.2$ , monoclinic,  $C2/c$ ,  $a = 11.768$  (2),  $b = 8.057$  (1),  $c = 21.363$  (4) Å,  $\beta = 106.83$  (1)°,  $U = 1938.7$  (4) Å<sup>3</sup>,  $Z = 8$ ,  $D_x = 1.344$  Mg m<sup>-3</sup>,  $\lambda(\text{Cu } K\alpha) = 1.54178$  Å,  $\mu = 0.727$  mm<sup>-1</sup>,  $F(000) = 816$ ,  $T = 293$  K, final  $R = 0.060$  for 1688 reflections. The dihedral angle between the pyridine and phenyl rings is 1.4 (1)°. An

\* Present address: Central Research Laboratories, SS Pharmaceutical Co., Ltd, 1143 Nanpeidai, Narita 286, Japan.