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The Crystal Structure of 2-(*o*-Hydroxyphenyl)benzothiazole

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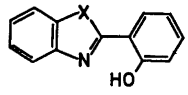
The crystal structure of 2-(*o*-hydroxyphenyl)benzothiazole consists of planar and discrete molecules $C_{13}H_9NOS$ with a shortest intermolecular distance (C – O) of 3.37 Å. There is a strong intramolecular chelating hydrogen bond O – H···N, with an O – N distance of 2.605 (9) Å.

X-Ray single crystal data (1078 reflections) have been refined to an *R*-value of 0.088. The crystals are monoclinic (space group $P2_1/c$) with $a = 12.423$ Å, $b = 5.858$ Å, $c = 15.624$ Å, and $\beta = 111.66°$.

2-(*o*-Hydroxyphenyl)benzoxazole (I) and 2-(*o*-hydroxyphenyl)benzothiazole (II) form insoluble chelates of analytical interest with some bivalent metal ions.



I: X = O
II: X = S

The crystal structure of the copper(II) chelate of I has been published earlier by the present author [1] and structure investigations of other metal chelates of I and II are in progress. In connection with this work the crystal structures of the pure organic chelating agents I and II have been studied. This paper presents a report on the crystal structure of II, which has been determined by X-ray methods. It will be followed by a similar report on compound I.

EXPERIMENTAL

Preparation. Compound II was prepared from *o*-aminothiophenol and salicylamide [2] and purified by vacuum distillation and recrystallizations from ethyl alcohol-water mixtures. Suitable single crystals were obtained from ethyl alcohol solutions as colourless plates.

Analysis. Elemental analyses were performed by AB Analytica, Sollentuna, Sweden. (Found: C 68.8; H 4.2; S 14.9. Calc.: C 68.7; H 4.0; S 14.1.)

STRUCTURE DETERMINATION

Cell dimensions and density. X-Ray powder diffraction photographs were recorded in a Guinier-Hägg focusing camera with Cu$K\alpha_1$ radiation. KCl was added as an internal standard. The following lattice parameters were calculated by the program PIRUM:

$$a = 12.423 \pm 0.002 \text{ Å},$$
$$b = 5.858 \pm 0.001 \text{ Å},$$
$$c = 15.624 \pm 0.004 \text{ Å},$$
$$\beta = 111.66 \pm 0.02°.$$

The density was determined by flotation to be 1.41 g/cm^3. Assuming a cell content of 4 formula units, the calculated density is 1.43 g/cm^3.

Single crystal work. Reflections *h*0*l* to *h*5*l* were recorded with an integrating Weissenberg camera, using Ni-filtered Cu$K\alpha$ radiation. The intensities of 1078 independent reflections were measured photometrically and corrected for Lorentz and polarization effects. The approximate dimensions of the single crystals were $0.3 \times 0.2 \times 0.01$ mm^3. The maximum absorption was found to be negligible ($\mu \times R = 0.5$), and thus no absorption correction was made.

Computer programs. Fig. 2 was drawn by the program OR TEP, written by C. K. Johnson, Oak Ridge, Tennessee. All the other computer programs used in this work have been listed elsewhere.[1]

Space group and atomic positions. The space group $P2_1/c$ was indicated by Weissenberg photographs with the crystal oriented along its *c*-axis (*hk*0). Reflections 0*k*0 were found only for $k = 2n$. The final recording along the *b*-axis (*h*0*l* – *h*5*l*) revealed that reflections *h*0*l* occur only for $l = 2n$ (Table 1). These observations excluded all space groups except $P2_1/c$ (No. 14).[3] The unit cell contains four molecules according to density measurements. Three-dimensional Patterson functions and generalized Patterson projections $P_1(uw) - P_5(uw)$ have been calculated on the basis of data *h*0*l* – *h*5*l*. The parameters of the "heavy" sulphur atom, which had been obtained from the Harker section $P(u\frac{1}{2}w)$ as well as from generalized projections, made it possible to determine approximate signs for a sufficient number of the reflections. A three-dimensional Fourier synthesis revealed the atomic parameters of all the atoms except hydrogen, the approximate positions of which were calculated on the basis of difference syntheses. Geometrical considerations had also to be taken into account, since the difference syntheses exhibited some pronounced residual peaks, which could not possibly be assigned to any hydrogen atoms.

On refining the parameters with the least-squares program LALS, an agreement factor $R = 0.104$ was achieved with isotropic temperature factors for all the atoms, and $R = 0.099$ when anisotropic temperature factors were introduced for the heavy sulphur atom. The final refinement, which included isotropic temperature factors for the hydrogen atoms and anisotropic ones for all the other atoms, resulted in a significant [5] reduction of R to 0.088. Individual weighting factors were applied to the $|F_o|$-values according to the scheme recommended by Cruickshank.[5] The refinement includes only reflections with a ratio $F_o:F_c$ of 0.33 – 3.00, but only one reflection was in this way omitted.

Table 1. Observed and calculated structure factors.

h	k	l	$\|F_o\|$	$\|F_c\|$	h	k	l	$\|F_o\|$	$\|F_c\|$	h	k	l	$\|F_o\|$	$\|F_c\|$	h	k	l	$\|F_o\|$	$\|F_c\|$
2	0	0	9.7	7.2	4	0	-6	28.5	27.0	6	1	5	12.7	11.9	2	1	-8	9.8	9.8
3	0	0	41.2	49.3	5	0	-6	15.0	13.8	7	1	5	17.6	17.4	3	1	-8	13.4	12.6
4	0	0	65.4	72.3	7	0	-6	36.7	38.9	0	1	6	44.0	42.3	4	1	-8	68.5	69.8
5	0	0	18.3	14.4	8	0	-6	37.7	38.6	1	1	6	36.1	37.5	5	1	-8	45.2	44.8
6	0	0	53.7	53.2	9	0	-6	27.7	28.0	2	1	6	38.4	42.5	6	1	-8	24.4	24.9
7	0	0	20.8	19.4	10	0	-6	12.6	12.4	3	1	6	13.0	13.0	7	1	-8	31.5	32.0
8	0	0	14.1	11.4	11	0	-6	25.9	27.4	4	1	6	21.0	21.4	8	1	-8	16.6	17.7
12	0	0	11.0	7.6	14	0	-6	11.1	10.9	5	1	6	26.3	28.1	9	1	-8	15.2	15.4
0	0	2	54.5	46.7	1	0	-8	17.2	17.8	0	1	7	13.6	13.4	1	1	-9	23.6	23.9
1	0	2	20.0	20.0	3	0	-8	19.8	17.4	2	1	7	27.7	28.3	2	1	-9	11.0	11.7
2	0	2	60.7	58.0	4	0	-8	22.7	19.5	3	1	7	12.6	10.2	4	1	-9	13.0	11.5
3	0	2	17.6	20.1	5	0	-8	14.9	8.6	2	1	8	15.3	12.8	5	1	-9	14.3	12.3
4	0	2	76.2	79.5	7	0	-8	31.1	33.6	4	1	8	16.0	18.0	10	1	-9	12.2	11.8
5	0	2	16.8	17.6	8	0	-8	7.2	7.4	5	1	8	11.9	10.5	1	1	-10	25.6	27.4
6	0	2	16.5	17.8	11	0	-8	12.2	9.8	6	1	8	11.5	8.3	2	1	-10	37.7	40.1
7	0	2	29.1	29.8	13	0	-8	20.3	22.9	7	1	8	20.9	19.8	3	1	-10	15.9	16.0
8	0	2	18.6	17.2	15	0	-8	9.4	8.6	1	1	9	21.4	19.9	4	1	-10	12.2	10.9
9	0	2	21.9	19.7	1	0	-10	26.9	25.9	3	1	9	10.9	10.2	5	1	-10	16.4	15.3
10	0	2	14.8	14.0	2	0	-10	30.2	28.5	5	1	9	21.4	22.1	6	1	-10	18.4	17.5
12	0	2	9.3	8.6	7	0	-10	23.7	24.8	0	1	10	20.2	20.3	7	1	-10	24.6	24.6
0	0	4	7.9	0.8 *	9	0	-10	26.7	28.4	1	1	10	8.9	10.6	8	1	-10	11.6	12.8
1	0	4	24.4	21.1	10	0	-10	13.5	12.5	2	1	10	16.9	16.2	9	1	-10	11.3	11.4
2	0	4	13.6	14.7	11	0	-10	10.9	11.0	3	1	10	11.4	10.4	10	1	-10	17.3	18.1
3	0	4	24.9	25.5	12	0	-10	14.0	16.1	5	1	10	9.0	8.2	11	1	-10	13.7	14.6
4	0	4	53.1	53.6	13	0	-10	25.9	29.8	2	1	11	15.6	14.4	1	1	-11	8.3	8.3
5	0	4	8.4	8.9	14	0	-10	7.2	6.9	0	1	12	11.4	14.0	2	1	-11	18.2	18.9
6	0	4	25.8	26.7	1	0	-12	20.2	22.0	1	1	12	13.7	13.0	3	1	-11	9.9	7.9
7	0	4	26.3	27.0	4	0	-12	12.1	14.2	2	1	12	26.7	30.9	4	1	-11	9.4	6.5
8	0	4	18.6	19.3	5	0	-12	8.2	6.7	3	1	12	21.3	22.3	8	1	-11	14.7	14.1
9	0	4	21.5	19.0	6	0	-12	24.7	21.3	5	1	12	12.0	12.3	1	1	-12	14.7	16.8
10	0	4	12.3	12.0	7	0	-12	27.2	25.9	1	1	13	11.6	12.1	2	1	-12	14.5	16.4
11	0	4	8.8	6.2	8	0	-12	21.7	22.1	3	1	13	11.1	12.9	5	1	-12	11.7	10.8
12	0	4	7.8	7.7	9	0	-12	25.6	26.8	2	1	-1	20.0	20.5	7	1	-12	10.2	6.0
0	0	6	43.7	41.8	10	0	-12	12.4	13.2	3	1	-1	27.5	27.9	3	1	-13	11.5	10.7
2	0	6	25.6	26.2	11	0	-12	12.3	14.0	4	1	-1	5.5	4.2					
3	0	6	16.3	16.8	12	0	-12	10.4	10.4	6	1	-1	17.9	17.5	1	2	0	34.5	38.0
4	0	6	9.5	6.7	2	0	-14	12.9	13.9	7	1	-1	15.6	11.7	2	2	0	23.8	25.6
6	0	6	9.3	7.8	3	0	-14	25.8	28.3	10	1	-1	12.8	9.5	3	2	0	40.0	45.9
7	0	6	25.4	27.0	4	0	-14	35.9	37.5	1	1	-2	17.0	15.9	4	2	0	13.0	16.7
8	0	6	9.2	9.5	5	0	-14	10.8	9.9	2	1	-2	43.4	43.3	5	2	0	30.7	33.1
9	0	6	14.8	14.2	7	0	-14	12.3	10.7	3	1	-2	8.4	7.3	6	2	0	18.7	17.5
0	0	8	25.1	27.1	8	0	-14	13.8	12.6	4	1	-2	29.6	30.7	7	2	0	18.4	16.0
1	0	8	39.9	40.4	9	0	-14	21.7	20.8	5	1	-2	35.1	39.2	10	2	0	6.5	5.7
2	0	8	20.5	20.2	10	0	-14	15.5	14.6	6	1	-2	53.0	57.6	11	2	0	9.6	9.2
3	0	8	21.2	22.5	10	0	-16	7.7	6.6	7	1	-2	29.9	31.5	0	2	1	21.2	25.6
4	0	8	32.8	34.4						8	1	-2	17.4	16.9	1	2	1	8.8	7.6
5	0	8	29.5	29.3	2	1	0	22.8	21.5	9	1	-2	35.2	33.5	2	2	1	29.7	31.4
6	0	8	12.3	13.2	3	1	0	20.7	18.9	11	1	-2	12.8	12.3	4	2	1	16.6	17.2
7	0	8	9.8	7.0	4	1	0	16.6	14.9	12	1	-2	16.4	14.9	5	2	1	16.9	16.5
8	0	8	8.8	6.6	5	1	0	7.1	6.7	1	1	-3	85.5	87.3	7	2	1	16.6	17.5
0	0	10	20.2	20.9	6	1	0	23.7	26.1	2	1	-3	82.7	83.4	8	2	1	23.1	23.6
1	0	10	12.6	14.4	8	1	0	30.9	25.1	4	1	-3	29.8	29.3	9	2	1	10.2	10.0
2	0	10	17.6	19.2	9	1	0	32.9	33.6	5	1	-3	7.0	7.3	10	2	1	12.4	13.5
3	0	10	18.5	19.9	10	1	0	20.5	19.6	6	1	-3	20.6	20.7	0	2	2	17.6	19.0
4	0	10	10.9	9.0	11	1	0	18.3	16.5	7	1	-3	18.2	18.0	2	2	2	41.7	39.8
5	0	10	9.0	9.0	12	1	0	10.7	7.7	8	1	-3	9.8	7.2	3	2	2	58.7	63.9
7	0	10	13.1	13.3	13	1	0	9.4	7.8	9	1	-3	8.9	9.1	4	2	2	37.3	40.9
8	0	10	6.0	6.8	1	1	1	21.4	23.0	10	1	-3	16.7	14.4	5	2	2	24.8	26.5
9	0	10	6.2	6.1	2	1	1	7.8	6.8	1	1	-4	37.0	36.7	6	2	2	25.8	25.7
0	0	12	9.0	8.6	4	1	1	10.7	10.6	2	1	-4	161.3	171.1	7	2	2	37.9	39.6
2	0	12	13.0	8.5	5	1	1	19.9	19.2	3	1	-4	60.0	58.1	8	2	2	7.4	6.7
3	0	12	13.0	8.1	6	1	1	9.2	6.1	5	1	-4	42.5	48.1	10	2	2	8.1	9.0
5	0	12	25.1	15.6	7	1	1	9.9	8.0	6	1	-4	22.5	25.5	11	2	2	9.8	10.2
6	0	12	13.4	5.1	9	1	1	10.1	7.4	7	1	-4	9.1	6.4	0	2	3	3.5	2.3
1	0	14	12.1	11.4	1	1	2	51.9	57.2	8	1	-4	15.5	16.6	1	2	3	22.2	22.5
2	0	14	15.5	17.4	2	1	2	15.1	16.5	9	1	-4	14.4	12.2	2	2	3	20.0	18.6
0	0	16	22.7	25.1	3	1	2	9.2	6.1	11	1	-4	16.1	16.0	3	2	3	7.3	6.1
1	0	16	7.5	9.3	4	1	2	17.4	17.6	1	1	-5	7.8	6.7	4	2	3	7.0	6.1
3	0	16	9.7	11.5	5	1	2	24.9	25.0	2	1	-5	11.3	11.0	7	2	3	11.4	9.3
2	0	-2	30.2	26.5	7	1	2	9.0	10.7	3	1	-5	58.6	61.3	0	2	4	7.1	3.6
3	0	-2	83.4	88.9	9	1	2	12.1	12.8	5	1	-5	8.2	8.3	1	2	4	13.3	13.2
4	0	-2	21.9	17.8	0	1	3	37.0	36.9	6	1	-5	15.8	13.6	2	2	4	16.8	13.7
7	0	-2	22.8	21.8	1	1	3	32.8	32.0	8	1	-5	16.7	16.0	3	2	4	13.5	14.3
8	0	-2	10.8	11.1	2	1	3	12.4	11.4	9	1	-5	14.8	13.5	6	2	4	22.3	23.2
9	0	-2	14.4	16.6	3	1	3	7.8	5.9	2	1	-6	15.0	13.1	7	2	4	26.6	26.5
10	0	-2	6.9	8.1	4	1	3	36.1	38.7	3	1	-6	8.0	8.8	8	2	4	11.4	11.5
15	0	-2	5.2	8.3	5	1	3	12.2	6.8	4	1	-6	8.8	8.0	9	2	4	19.2	19.9
1	0	-4	33.1	28.6	7	1	3	9.4	8.8	5	1	-6	45.6	49.5	10	2	4	10.5	7.9
2	0	-4	200.1	186.9	9	1	3	13.4	12.2	6	1	-6	10.3	7.6	11	2	4	8.8	8.2
3	0	-4	48.8	44.9	0	1	4	7.4	8.6	7	1	-6	23.8	23.5	0	2	5	10.7	9.0
4	0	-4	25.2	22.9	1	1	4	28.9	34.0	8	1	-6	9.0	8.3	1	2	5	23.9	22.6
5	0	-4	32.0	28.3	2	1	4	43.7	49.5	10	1	-6	14.8	16.2	3	2	5	12.6	12.0
6	0	-4	30.1	27.7	3	1	4	14.1	15.5	11	1	-6	25.3	28.9	5	2	5	12.1	13.1
10	0	-4	18.2	17.9	5	1	4	22.4	22.0	1	1	-7	7.3	8.3	7	2	5	14.5	15.2
11	0	-4	29.5	29.2	6	1	4	23.7	23.7	2	1	-7	8.0	6.6	0	2	6	27.6	27.8
12	0	-4	16.4	16.9	7	1	4	22.2	17.7	3	1	-7	35.5	34.4	1	2	6	39.3	37.7
13	0	-4	13.2	14.3	8	1	4	12.4	10.8	4	1	-7	29.5	28.2	2	2	6	22.1	23.6
15	0	-4	6.9	6.7	1	1	5	26.7	22.7	5	1	-7	13.9	15.3	3	2	6	17.2	17.9
1	0	-6	40.8	40.2	2	1	5	12.1	11.3	6	1	-7	19.0	18.7	4	2	6	8.5	6.6
2	0	-6	7.3	4.5	3	1	5	32.5	32.1	7	1	-7	9.7	7.7	5	2	6	18.9	16.6
3	0	-6	15.4	11.9	5	1	5	9.3	6.5	9	1	-7	13.5	10.6	6	2	6	12.9	14.7

Table 1. Continued.

h	k	l	$\|F_o\|$	$\|F_c\|$
10	2	6	9.0	8.8
0	2	7	35.8	36.7
1	2	7	6.6	7.2
2	2	7	17.9	16.5
4	2	7	16.4	16.6
0	2	8	26.4	27.9
2	2	8	5.3	5.9
3	2	8	11.9	12.9
4	2	8	23.8	25.0
5	2	8	23.3	23.3
6	2	8	9.3	8.5
7	2	8	9.0	9.5
0	2	9	15.3	15.3
1	2	9	15.7	15.9
3	2	9	16.2	17.1
4	2	9	16.8	19.7
0	2	10	8.8	8.8
2	2	10	11.4	11.6
4	2	10	14.0	14.7
5	2	10	11.4	11.6
6	2	10	8.2	8.4
7	2	10	9.5	7.2
8	2	10	9.5	12.4
0	2	11	10.3	9.6
1	2	11	7.2	8.9
3	2	11	8.1	8.6
6	2	11	5.5	6.4
1	2	12	7.4	4.1
5	2	12	5.9	6.3
6	2	12	6.2	4.4
0	2	13	5.6	4.8
2	2	13	7.4	9.0
3	2	13	5.5	6.2
0	2	14	7.4	7.4
2	2	14	6.4	4.7
3	2	14	8.8	8.8
4	2	14	8.3	6.0
0	2	15	6.0	9.1
0	2	16	7.5	8.4
1	2	16	8.8	10.5
2	2	16	5.1	7.6
1	2	-1	16.7	17.7
2	2	-1	15.0	14.4
3	2	-1	27.4	27.8
4	2	-1	22.4	22.0
5	2	-1	9.4	9.2
7	2	-1	6.3	4.3
8	2	-1	10.7	9.9
9	2	-1	17.6	18.7
11	2	-1	12.1	11.9
2	2	-2	14.3	12.8
3	2	-2	43.8	44.7
4	2	-2	4.3	3.2
5	2	-2	25.9	25.0
8	2	-2	15.5	16.2
9	2	-2	25.3	27.9
13	2	-2	8.5	9.5
1	2	-3	14.5	14.4
4	2	-8	64.3	61.0
5	2	-8	27.5	23.8
6	2	-8	4.9	3.9
8	2	-8	5.8	6.5
9	2	-8	6.7	4.5
10	2	-8	11.0	9.7
11	2	-8	8.2	6.3
12	2	-8	5.5	4.6
2	2	-9	11.3	9.9
5	2	-9	32.2	30.1
7	2	-9	15.0	14.7
9	2	-9	6.1	5.3
10	2	-9	8.2	6.9
11	2	-9	13.6	14.7
1	2	-10	7.4	6.1
2	2	-10	15.1	12.8
3	2	-10	6.3	5.1
5	2	-10	13.9	12.9
6	2	-10	7.5	6.1
8	2	-10	14.6	13.5
9	2	-10	9.4	7.9
10	2	-10	14.1	14.2
11	2	-10	14.8	16.2
12	2	-10	11.4	12.1
13	2	-10	8.3	7.5
14	2	-10	5.9	5.3
5	2	-11	14.0	12.8
6	2	-11	20.2	18.6
7	2	-11	9.8	7.1
8	2	-11	8.6	6.2
9	2	-11	6.5	6.1
1	2	-12	7.0	6.0
2	2	-12	10.8	11.9
3	2	-12	6.5	7.0
5	2	-12	7.0	5.4
6	2	-12	42.5	40.9
7	2	-12	30.8	27.9
8	2	-12	10.3	8.0
9	2	-12	12.5	12.0
10	2	-12	11.3	13.2
11	2	-12	6.0	8.1
1	2	-13	10.1	9.4
5	2	-13	7.1	5.5
6	2	-13	11.2	9.8
9	2	-13	6.0	5.1
11	2	-13	5.9	6.7
12	2	-13	8.5	9.9
13	2	-13	6.3	7.1
1	2	-14	6.7	4.2
2	2	-14	11.3	12.1
3	2	-14	15.9	16.6
4	2	-14	21.4	21.8
5	2	-14	16.7	16.6
6	2	-14	15.4	14.7
7	2	-14	17.2	16.4
9	2	-14	6.0	7.3
3	2	-15	7.4	7.8
4	2	-15	12.2	12.8
5	2	-15	9.9	8.1
7	2	-15	7.9	6.1
2	2	-3	27.7	27.0
3	2	-3	32.2	32.6
4	2	-3	28.3	26.8
5	2	-3	18.1	17.3
6	2	-3	8.5	5.7
7	2	-3	6.8	4.9
8	2	-3	8.6	10.5
9	2	-3	18.8	20.4
10	2	-3	20.8	20.7
12	2	-3	13.5	13.9
13	2	-3	6.4	6.8
2	2	-4	12.4	11.6
3	2	-4	21.9	19.2
4	2	-4	34.0	33.6
5	2	-4	29.6	29.3
6	2	-4	10.5	11.4
7	2	-4	26.2	27.5
8	2	-4	22.6	23.7
9	2	-4	5.5	6.2
10	2	-4	5.8	6.2
11	2	-4	16.8	13.9
12	2	-4	13.7	14.1
13	2	-4	5.8	4.9
14	2	-4	8.1	8.3
1	2	-5	9.3	10.4
2	2	-5	4.6	3.9
3	2	-5	42.5	40.2
4	2	-5	6.1	4.7
5	2	-5	9.5	9.1
6	2	-5	15.1	13.8
7	2	-5	8.0	8.1
8	2	-5	5.9	7.1
9	2	-5	9.7	9.7
13	2	-5	6.4	6.2
1	2	-6	13.8	14.7
2	2	-6	21.5	21.3
3	2	-6	4.8	3.2
4	2	-6	24.0	22.4
5	2	-6	28.9	26.4
6	2	-6	27.9	28.6
7	2	-6	11.6	12.7
8	2	-6	26.1	27.1
9	2	-6	21.8	22.3
10	2	-6	10.4	10.0
13	2	-6	9.1	9.1
14	2	-6	6.2	6.3
1	2	-7	20.4	19.7
2	2	-7	19.1	19.6
3	2	-7	39.7	36.9
4	2	-7	59.6	55.9
5	2	-7	16.6	14.5
6	2	-7	13.6	12.3
7	2	-7	7.5	6.3
8	2	-7	12.7	13.0
10	2	-7	5.4	5.0
11	2	-7	4.8	4.7
12	2	-7	9.4	8.4
1	2	-8	9.5	9.5
2	2	-8	16.8	16.2
3	2	-8	23.3	20.9
2	2	-16	9.5	11.0
3	2	-16	11.8	12.6
6	2	-16	10.0	9.2
7	2	-16	9.1	8.4
8	2	-16	10.2	10.3
9	2	-16	7.7	6.6
6	2	-17	8.0	7.8
7	2	-17	8.0	9.2
8	2	-17	6.3	6.7
6	2	-18	5.4	6.1
7	2	-18	8.3	8.7
8	2	-18	8.7	9.3
9	2	-18	7.2	7.6
1	3	0	18.7	24.0
2	3	0	23.6	26.0
3	3	0	6.2	3.9
4	3	0	9.2	9.0
5	3	0	14.9	14.8
9	3	0	16.6	16.8
10	3	0	11.2	10.8
11	3	0	12.2	9.9
12	3	0	10.4	10.6
0	3	1	9.7	12.3
1	3	1	19.1	22.7
2	3	1	27.3	31.1
3	3	1	23.4	24.1
5	3	1	11.7	10.5
7	3	1	22.2	27.1
8	3	1	19.3	21.8
9	3	1	13.5	10.3
10	3	1	12.7	8.7
0	3	2	23.7	25.6
1	3	2	21.7	23.4
2	3	2	7.5	6.7
3	3	2	19.7	21.1
4	3	2	9.4	11.1
6	3	2	9.0	9.4
9	3	2	14.9	13.2
0	3	3	8.3	7.4
1	3	3	18.1	19.2
2	3	3	35.0	39.4
3	3	3	11.6	10.1
4	3	3	13.8	7.9
6	3	3	18.0	18.1
7	3	3	18.1	17.6
8	3	3	14.8	10.7
0	3	4	33.9	34.5
1	3	4	15.6	17.6
2	3	4	11.0	11.6
3	3	4	18.6	17.8
4	3	4	15.8	17.2
5	3	4	11.8	10.9
7	3	4	15.8	14.2
0	3	5	25.3	25.4
1	3	5	12.4	13.0
2	3	5	16.8	18.5
3	3	5	11.4	11.8
5	3	5	25.6	27.6
6	3	5	26.2	30.6
8	3	5	13.6	10.7
0	3	6	25.2	25.2
1	3	6	21.3	22.2
2	3	6	15.8	15.7
3	3	6	11.1	12.4
4	3	6	20.7	21.4
5	3	6	13.6	12.0
7	3	6	14.6	11.8
8	3	6	13.7	12.6
9	3	6	10.1	10.6
5	3	7	15.3	16.2
6	3	7	11.6	10.7
4	3	9	11.4	11.8
0	3	10	16.6	19.8
0	3	11	12.1	13.3
0	3	12	13.5	11.8
3	3	12	9.2	11.7
1	3	-1	14.4	17.6
3	3	-1	12.3	12.0
4	3	-1	28.6	30.2
5	3	-1	16.4	18.8
6	3	-1	13.0	16.0
8	3	-1	10.1	9.4
1	3	-2	7.6	7.7
2	3	-2	13.6	14.6
3	3	-2	26.0	26.8
4	3	-2	29.9	31.9
5	3	-2	33.4	36.5
6	3	-2	22.4	25.2
7	3	-2	21.5	23.1
8	3	-2	15.5	16.3
9	3	-2	10.2	8.3
1	3	-3	18.9	17.8
2	3	-3	28.5	27.4
3	3	-3	16.3	15.1
4	3	-3	15.1	15.1
6	3	-3	13.5	12.7
7	3	-3	18.8	19.2
11	3	-3	12.9	10.7
1	3	-4	27.1	26.7
2	3	-4	24.9	23.4
3	3	-4	11.8	11.4
4	3	-4	7.8	8.0
5	3	-4	8.9	7.3
6	3	-4	8.5	7.1
7	3	-4	9.1	9.0
8	3	-4	12.5	13.7
9	3	-4	12.7	12.0
10	3	-4	10.6	10.5
2	3	-5	10.4	5.5
5	3	-5	17.6	18.8
7	3	-5	11.2	7.9
9	3	-5	12.9	11.0
13	3	-5	8.5	8.4
2	3	-6	8.3	5.6
3	3	-6	11.5	10.2
5	3	-6	7.5	5.8
6	3	-6	11.8	8.2
7	3	-6	11.8	9.2
8	3	-6	13.9	14.6
9	3	-6	14.6	15.8
10	3	-6	13.5	13.3
1	3	-7	16.8	12.5
3	3	-7	13.3	10.7
4	3	-7	13.5	11.4
6	3	-7	8.5	6.3
7	3	-7	9.2	6.2
9	3	-7	16.6	17.6
10	3	-7	10.6	9.2
1	3	-8	11.4	8.3
4	3	-8	16.3	14.7
5	3	-8	9.7	8.1
6	3	-8	13.1	11.9
7	3	-8	12.8	11.7
8	3	-8	13.9	14.5
9	3	-8	13.1	13.8
10	3	-8	11.3	12.9
11	3	-8	14.9	14.7
12	3	-8	12.4	12.7
13	3	-8	10.1	10.9
2	3	-9	12.8	8.8
3	3	-9	9.2	6.7
5	3	-9	26.1	25.0
8	3	-9	10.5	9.5
9	3	-9	11.4	11.3
1	3	-10	21.5	22.5
2	3	-10	26.7	23.9
3	3	-10	20.0	19.2
4	3	-10	26.0	26.3
5	3	-10	12.3	9.0
7	3	-10	14.0	11.0
8	3	-10	12.1	9.4
1	3	-11	13.4	10.0
2	3	-11	22.0	23.8
3	3	-11	18.1	16.6
5	3	-11	31.3	28.9
6	3	-11	31.8	30.8
9	3	-12	11.4	8.8
4	3	-12	16.3	16.9
5	3	-12	15.5	15.5
6	3	-12	12.9	8.5
7	3	-12	15.1	15.2
1	3	-13	13.9	11.2
4	3	-13	14.1	11.9
5	3	-13	16.0	13.1
7	3	-13	17.2	18.1
5	3	-14	10.2	12.0
6	3	-14	10.9	12.3
2	3	-15	10.7	9.8
7	3	-15	14.5	13.9
8	3	-15	16.6	17.5
7	3	-16	9.8	10.0
8	3	-16	11.7	12.5
9	3	-16	13.5	14.8
10	3	-16	9.9	8.3
1	4	0	8.7	11.7
2	4	0	13.5	14.8
4	4	0	5.5	5.7
5	4	0	6.2	4.8
6	4	0	12.6	12.8
7	4	0	11.9	12.9
8	4	0	14.2	13.1
9	4	0	13.8	13.1
0	4	1	8.7	11.6
1	4	1	11.2	13.2

Table 1. Continued.

h	k	l	$\|F_o\|$	$\|F_c\|$	h	k	l	$\|F_o\|$	$\|F_c\|$	h	k	l	$\|F_o\|$	$\|F_c\|$	h	k	l	$\|F_o\|$	$\|F_c\|$
2	4	1	7.1	6.3	5	4	-3	5.8	5.1	5	5	0	3.6	3.3	2	5	-2	8.7	9.1
3	4	1	4.5	6.0	6	4	-3	8.6	7.5	6	5	0	6.8	5.9	3	5	-2	16.4	16.3
4	4	1	17.4	18.2	7	4	-3	11.4	10.3	7	5	0	9.4	8.8	4	5	-2	16.8	15.0
5	4	1	16.2	16.7	9	4	-3	7.3	5.7	8	5	0	3.9	3.3	5	5	-2	10.2	9.6
6	4	1	9.6	10.1	10	4	-3	11.4	11.5	9	5	0	3.2	3.8	7	5	-2	8.8	8.0
7	4	1	5.9	4.1	12	4	-3	5.0	6.7	10	5	0	6.0	5.8	8	5	-2	6.6	5.8
8	4	1	12.8	11.8	1	4	-4	13.8	13.1	0	5	1	5.2	7.3	1	5	-3	20.5	24.6
9	4	1	7.5	5.4	2	4	-4	14.3	16.0	1	5	1	12.5	12.7	2	5	-3	9.4	8.4
10	4	1	8.2	5.5	4	4	-4	12.3	10.3	2	5	1	11.4	10.3	3	5	-3	4.1	3.8
0	4	2	12.6	13.3	6	4	-4	11.1	11.4	3	5	1	4.6	3.2	5	5	-3	3.5	3.2
1	4	2	23.4	23.2	7	4	-4	7.4	6.2	5	5	1	11.5	10.3	6	5	-3	6.1	6.2
2	4	2	26.2	26.9	9	4	-4	12.4	13.8	9	5	1	4.2	4.3	7	5	-3	5.7	4.7
3	4	2	17.2	17.9	10	4	-4	11.1	11.6	10	5	1	5.8	6.4	8	5	-3	11.7	11.8
4	4	2	14.8	14.6	11	4	-4	11.6	12.9	0	5	2	14.9	20.6	9	5	-3	7.5	6.7
5	4	2	18.2	17.4	12	4	-4	7.8	8.2	1	5	2	11.1	11.4	10	5	-3	7.5	7.4
6	4	2	14.7	13.5	13	4	-4	4.6	5.6	2	5	2	13.8	14.4	11	5	-3	3.0	3.0
8	4	2	9.5	6.3	2	4	-5	6.5	6.9	3	5	2	11.8	10.7	1	5	-4	7.3	8.0
9	4	2	9.6	8.3	3	4	-5	21.7	20.8	5	5	2	9.3	8.4	2	5	-4	5.0	4.1
10	4	2	8.1	7.3	5	4	-5	9.6	10.0	6	5	2	7.1	6.5	3	5	-4	14.5	15.1
1	4	3	14.2	13.6	6	4	-5	20.6	21.7	8	5	2	6.4	6.1	4	5	-4	9.2	9.2
2	4	3	17.7	17.1	7	4	-5	20.3	22.7	9	5	2	7.2	8.1	7	5	-4	6.1	4.7
3	4	3	12.8	13.3	8	4	-5	12.5	12.8	0	5	3	11.4	10.9	8	5	-4	3.4	3.5
7	4	3	6.7	5.2	9	4	-5	8.1	6.3	1	5	3	15.8	17.0	10	5	-4	5.8	4.2
8	4	3	8.4	7.2	10	4	-5	12.1	13.0	2	5	3	18.3	19.4	11	5	-4	4.7	5.2
10	4	3	8.0	8.8	11	4	-5	7.0	5.7	3	5	3	15.3	14.7	1	5	-5	21.1	23.3
11	4	3	6.9	7.5	1	4	-6	28.1	27.9	4	5	3	6.4	5.9	2	5	-5	5.0	5.2
0	4	4	19.2	17.8	2	4	-6	35.2	33.7	5	5	3	6.2	4.8	4	5	-5	12.3	12.3
3	4	4	12.5	13.0	3	4	-6	13.9	11.5	6	5	3	8.9	8.1	2	5	-6	5.9	5.6
5	4	4	6.0	5.9	5	4	-6	13.5	13.9	0	5	4	17.1	17.0	5	5	-6	6.3	6.6
6	4	4	8.9	7.2	6	4	-6	13.9	11.8	1	5	4	5.7	5.1	7	5	-6	4.4	3.8
7	4	4	5.4	4.9	7	4	-6	17.4	17.4	2	5	4	3.2	2.8	9	5	-6	8.9	9.3
8	4	4	8.3	7.0	9	4	-6	7.7	7.3	3	5	4	4.3	3.4	10	5	-6	6.1	6.2
10	4	4	7.3	8.3	10	4	-6	7.7	7.0	4	5	4	16.1	16.2	1	5	-7	4.6	4.4
1	4	5	9.1	8.1	13	4	-6	4.7	7.2	5	5	4	11.0	9.0	3	5	-7	4.9	3.7
2	4	5	7.5	7.9	1	4	-7	22.4	21.8	6	5	4	6.1	5.1	5	5	-7	4.5	2.7
5	4	5	11.4	10.9	3	4	-7	31.4	30.5	7	5	4	8.1	6.5	6	5	-7	4.4	3.5
0	4	6	18.8	19.4	4	4	-7	18.9	15.9	8	5	4	4.9	4.3	8	5	-7	5.4	4.8
1	4	6	17.0	16.7	6	4	-7	8.1	6.9	0	5	5	20.6	21.6	9	5	-7	3.8	4.5
2	4	6	14.2	12.9	10	4	-7	7.7	8.5	1	5	5	11.6	11.4	10	5	-7	6.1	7.0
4	4	6	6.7	6.7	1	4	-8	12.1	12.5	2	5	5	9.6	8.5	11	5	-7	4.4	6.5
0	4	7	27.5	27.8	2	4	-8	30.5	29.7	3	5	5	17.8	17.9	5	5	-8	10.6	8.9
1	4	7	16.4	17.2	3	4	-8	19.5	19.0	4	5	5	9.9	9.3	6	5	-8	12.8	10.2
4	4	7	10.6	9.0	4	4	-8	9.2	5.9	6	5	5	4.2	2.4	7	5	-8	8.8	8.7
1	4	8	12.4	13.0	5	4	-8	13.3	12.5	7	5	5	5.3	5.2	8	5	-8	5.5	4.5
2	4	8	18.6	19.2	6	4	-8	7.6	7.8	8	5	5	6.4	6.8	9	5	-8	4.3	4.2
4	4	8	7.5	6.5	1	4	-9	12.2	12.4	0	5	6	3.6	4.9	10	5	-8	3.5	4.0
5	4	8	9.7	7.6	2	4	-9	10.7	9.5	1	5	6	6.4	6.1	11	5	-8	5.8	6.4
6	4	8	8.5	6.9	3	4	-9	12.8	12.1	2	5	6	9.5	7.8	1	5	-9	5.3	4.3
0	4	9	6.3	5.5	5	4	-9	7.2	6.9	3	5	6	13.3	13.6	2	5	-9	11.4	11.2
1	4	9	11.5	12.9	6	4	-9	9.7	9.8	4	5	6	10.2	11.1	3	5	-9	13.6	12.5
2	4	9	7.3	6.2	1	4	-10	8.4	6.8	5	5	6	5.4	6.4	4	5	-9	9.0	7.7
3	4	9	15.2	13.1	3	4	-10	18.0	15.5	6	5	6	7.6	8.7	5	5	-9	8.0	6.4
4	4	9	9.8	8.3	4	4	-10	15.9	13.0	7	5	6	6.7	6.8	6	5	-9	6.8	7.4
6	4	9	8.8	9.3	7	4	-10	6.9	7.8	8	5	6	3.9	3.9	7	5	-9	5.9	5.8
7	4	9	5.6	5.3	9	4	-10	6.5	5.0	1	5	7	3.7	3.0	8	5	-9	13.8	13.3
1	4	10	11.2	8.6	11	4	-10	6.3	8.5	5	5	7	7.4	7.1	9	5	-9	10.7	10.3
2	4	10	15.8	15.7	12	4	-10	6.4	8.1	6	5	7	4.8	6.6	10	5	-9	7.0	8.6
3	4	10	11.4	12.5	2	4	-11	6.2	6.8	0	5	8	4.7	3.1	11	5	-9	5.0	6.2
5	4	10	5.7	7.4	3	4	-11	7.8	7.8	1	5	8	4.6	3.8	1	5	-10	6.6	6.7
6	4	10	7.7	6.7	5	4	-11	9.6	8.7	2	5	8	6.5	5.7	3	5	-10	10.2	9.0
3	4	11	12.4	12.7	11	4	-11	5.5	6.5	3	5	8	5.3	3.7	4	5	-10	12.3	10.4
4	4	11	6.2	6.7	12	4	-11	6.8	8.2	4	5	8	3.4	3.7	5	5	-10	4.0	3.7
6	4	11	4.8	5.5	3	4	-12	5.5	6.6	5	5	8	2.1	2.4	6	5	-10	4.6	3.1
0	4	12	7.3	7.7	4	4	-12	8.5	9.3	0	5	9	7.4	5.3	7	5	-10	9.3	8.5
0	4	14	6.3	7.3	5	4	-12	9.8	8.8	1	5	9	7.8	7.2	8	5	-10	7.6	8.1
1	4	14	8.0	8.9	8	4	-12	10.1	10.6	3	5	9	8.1	9.3	9	5	-10	5.7	6.5
1	4	-1	5.2	6.9	9	4	-12	10.0	9.9	4	5	9	2.7	2.9	10	5	-10	3.7	3.9
2	4	-1	4.9	4.2	10	4	-12	7.2	6.9	0	5	10	7.7	7.6	1	5	-11	6.8	7.3
3	4	-1	10.3	11.3	11	4	-12	4.4	6.5	1	5	10	7.4	6.8	2	5	-11	9.1	8.4
4	4	-1	12.8	13.7	12	4	-12	5.6	7.9	3	5	10	4.6	5.0	3	5	-11	9.7	7.5
5	4	-1	7.9	7.2	1	4	-13	8.8	6.9	4	5	10	6.5	6.1	4	5	-11	8.1	6.8
6	4	-1	10.1	10.0	3	4	-13	7.2	6.9	0	5	11	4.4	5.4	5	5	-11	9.2	7.9
7	4	-1	10.7	9.9	4	4	-13	6.8	7.3	1	5	11	2.8	3.3	6	5	-11	7.5	6.0
8	4	-1	10.5	10.1	5	4	-13	7.1	5.9	2	5	11	4.1	4.2	7	5	-11	5.5	5.7
12	4	-1	7.2	6.7	7	4	-13	5.5	6.1	0	5	12	5.8	6.6	8	5	-11	9.9	10.3
1	4	-2	9.3	11.0	8	4	-13	8.9	7.6	0	5	13	7.6	8.7	9	5	-11	3.8	4.2
2	4	-2	7.6	8.1	10	4	-13	4.9	5.6	1	5	13	9.4	13.2	1	5	-12	4.4	5.2
3	4	-2	7.4	6.3	1	4	-14	7.6	9.1	1	5	-1	23.0	23.4	2	5	-12	4.6	3.3
4	4	-2	6.0	3.8	2	4	-14	9.0	10.4	2	5	-1	3.4	2.2	3	5	-12	5.6	4.9
5	4	-2	11.3	12.0	3	4	-14	7.9	8.8	3	5	-1	12.6	12.9	4	5	-12	10.4	9.4
6	4	-2	7.5	7.1	9	4	-14	6.0	5.6	4	5	-1	20.5	19.9	5	5	-12	8.3	6.9
7	4	-2	13.0	13.6	10	4	-14	5.4	6.9	5	5	-1	19.4	19.2	6	5	-12	4.7	4.5
8	4	-2	10.0	8.8	7	4	-15	7.0	6.8	6	5	-1	5.3	4.7	7	5	-12	3.8	3.2
10	4	-2	7.4	7.2	8	4	-15	8.2	9.8	7	5	-1	4.3	5.7	9	5	-12	4.8	5.5
11	4	-2	13.3	14.3	8	4	-16	5.8	7.4	8	5	-1	9.3	10.0	1	5	-13	3.9	3.8
12	4	-2	4.4	4.0						9	5	-1	6.5	6.3	2	5	-13	3.1	2.8
1	4	-3	20.7	21.6	2	5	0	10.4	9.9	10	5	-1	6.7	7.0	3	5	-13	6.7	5.6
2	4	-3	8.8	7.4	3	5	0	3.2	3.0	11	5	-1	3.9	4.6	2	5	-14	2.8	2.2
3	4	-3	6.2	4.4	4	5	0	4.2	3.2	1	5	-2	6.7	8.2					

Table 2. Final atomic coordinates with standard deviations in parentheses.

	x	y	z
C(1)	0.3045 (8)	0.8000 (15)	0.2449 (6)
C(2)	0.4223 (9)	0.8055 (17)	0.3059 (7)
C(3)	0.4610 (9)	0.9783 (18)	0.3667 (7)
C(4)	0.3931 (8)	0.1545 (18)	0.3728 (7)
C(5)	0.2814 (7)	0.1602 (15)	0.3131 (6)
C(6)	0.2353 (6)	0.9877 (13)	0.2490 (5)
C(7)	0.1128 (7)	0.9916 (12)	0.1849 (5)
C(8)	0.9093 (6)	0.0812 (13)	0.0973 (5)
C(9)	0.7947 (8)	0.1528 (14)	0.0523 (6)
C(10)	0.7228 (7)	0.0127 (14)	0.9844 (6)
C(11)	0.7633 (7)	0.8132 (14)	0.9626 (6)
C(12)	0.8761 (7)	0.7410 (15)	0.0093 (6)
C(13)	0.9493 (6)	0.8780 (12)	0.0769 (5)
O	0.2684 (5)	0.6326 (10)	0.1861 (4)
S	0.0225 (2)	0.2208 (3)	0.1845 (1)
N	0.0667 (5)	0.8316 (10)	0.1271 (4)
H(2)	0.469 (8)	0.687 (17)	0.318 (7)
H(3)	0.535 (8)	0.986 (14)	0.410 (6)
H(4)	0.417 (7)	0.308 (15)	0.413 (6)
H(5)	0.239 (8)	0.300 (15)	0.327 (6)
H(9)	0.775 (7)	0.281 (13)	0.082 (5)
H(10)	0.646 (9)	0.058 (17)	0.952 (7)
H(11)	0.719 (6)	0.699 (11)	0.916 (5)
H(12)	0.918 (5)	0.602 (11)	0.998 (4)

Table 3. Temperature parameters. The parameters β_{ij} (standard deviations in parentheses) for carbon, nitrogen, oxygen, and sulphur have been based on the expression

$$\exp[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+hk\beta_{12}+hl\beta_{13}+kl\beta_{23})].$$

The parameters B (Å^2) for hydrogen have standard deviations of 1 – 2 Å^2.

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(1)	0.0083 (8)	0.0355 (30)	0.0039 (4)	0.0016 (23)	0.0037 (9)	−0.0002 (18)
C(2)	0.0094 (9)	0.0378 (35)	0.0058 (6)	0.0148 (28)	0.0044 (12)	−0.0009 (22)
C(3)	0.0069 (8)	0.0465 (40)	0.0059 (6)	0.0040 (28)	0.0025 (11)	−0.0036 (25)
C(4)	0.0073 (9)	0.0433 (36)	0.0064 (6)	−0.0045 (26)	0.0049 (12)	−0.0082 (23)
C(5)	0.0068 (7)	0.0336 (30)	0.0053 (5)	−0.0001 (22)	0.0056 (10)	−0.0028 (19)
C(6)	0.0054 (6)	0.0342 (27)	0.0033 (4)	0.0021 (19)	0.0036 (8)	0.0016 (16)
C(7)	0.0073 (7)	0.0214 (23)	0.0040 (4)	−0.0027 (17)	0.0056 (8)	−0.0013 (14)
C(8)	0.0057 (6)	0.0262 (24)	0.0036 (4)	−0.0014 (18)	0.0038 (8)	−0.0016 (14)
C(9)	0.0100 (9)	0.0283 (28)	0.0043 (5)	0.0034 (23)	0.0073 (10)	0.0014 (17)
C(10)	0.0055 (7)	0.0331 (28)	0.0043 (4)	−0.0015 (21)	0.0036 (9)	0.0005 (18)
C(11)	0.0061 (7)	0.0311 (28)	0.0051 (5)	−0.0076 (21)	0.0043 (9)	−0.0038 (18)
C(12)	0.0075 (7)	0.0297 (28)	0.0049 (5)	−0.0046 (23)	0.0054 (9)	−0.0013 (19)
C(13)	0.0064 (7)	0.0239 (23)	0.0035 (4)	−0.0038 (18)	0.0043 (8)	0.0003 (14)
O	0.0102 (6)	0.0348 (21)	0.0052 (4)	0.0101 (18)	0.0041 (8)	−0.0035 (14)
S	0.0067 (2)	0.0213 (6)	0.0040 (1)	0.0014 (5)	0.0047 (2)	−0.0021 (4)
N	0.0063 (6)	0.0270 (20)	0.0039 (3)	0.0007 (16)	0.0046 (7)	0.0003 (13)

	B		B
H(2)	3.0	H(9)	0.9
H(3)	2.1	H(10)	3.7
H(4)	2.3	H(11)	−0.4
H(5)	2.2	H(12)	−0.7

Table 4. Selected interatomic distances (Å) and angles (°) with estimated standard deviations.

O–C(1)	1.305	(11)	C(1)–C(2)–C(3)	120.0	(9)
C(1)–C(2)	1.422	(13)	C(2)–C(3)–C(4)	123.4	(10)
C(2)–C(3)	1.349	(15)	C(3)–C(4)–C(5)	118.3	(9)
C(3)–C(4)	1.359	(14)	C(4)–C(5)–C(6)	121.5	(8)
C(4)–C(5)	1.356	(13)	C(5)–C(6)–C(1)	120.3	(7)
C(5)–C(6)	1.389	(12)	C(6)–C(1)–C(2)	116.4	(8)
C(6)–C(1)	1.411	(12)	C(13)–C(8)–C(9)	122.1	(7)
C(6)–C(7)	1.481	(11)	C(8)–C(9)–C(10)	117.3	(8)
C(7)–S	1.749	(8)	C(9)–C(10)–C(11)	120.6	(8)
C(7)–N	1.280	(9)	C(10)–C(11)–C(12)	121.6	(8)
S–C(8)	1.757	(8)	C(11)–C(12)–C(13)	118.8	(8)
N–C(13)	1.404	(10)	C(12)–C(13)–C(8)	119.5	(7)
C(8)–C(9)	1.399	(12)	S–C(7)–N	116.1	(6)
C(9)–C(10)	1.377	(12)	C(7)–S–C(8)	88.6	(4)
C(10)–C(11)	1.365	(12)	S–C(8)–C(13)	109.2	(6)
C(11)–C(12)	1.386	(11)	N–C(13)–C(8)	115.4	(7)
C(12)–C(13)	1.369	(11)	C(7)–N–C(13)	110.8	(6)
C(13)–C(8)	1.372	(10)	C(5)–C(6)–C(7)	121.6	(7)
O–N	2.605	(9)	C(6)–C(7)–S	120.8	(5)
			O–C(1)–C(2)	119.3	(8)
H(2) –C(2)	0.88	(9)			
H(3) –C(3)	0.92	(9)			
H(4) –C(4)	1.07	(9)			
H(5) –C(5)	1.04	(9)			
H(9) –C(9)	0.96	(8)			
H(10)–C(10)	0.94	(10)			
H(11)–C(11)	0.99	(7)			
H(12)–C(12)	1.02	(6)			

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

Observed and calculated structure factors are listed in Table 1, and final coordinates and thermal parameters with standard deviations are given in Tables 2 and 3. Selected interatomic distances and bond angles including standard deviations are listed in Table 4 and also shown in Fig. 1.

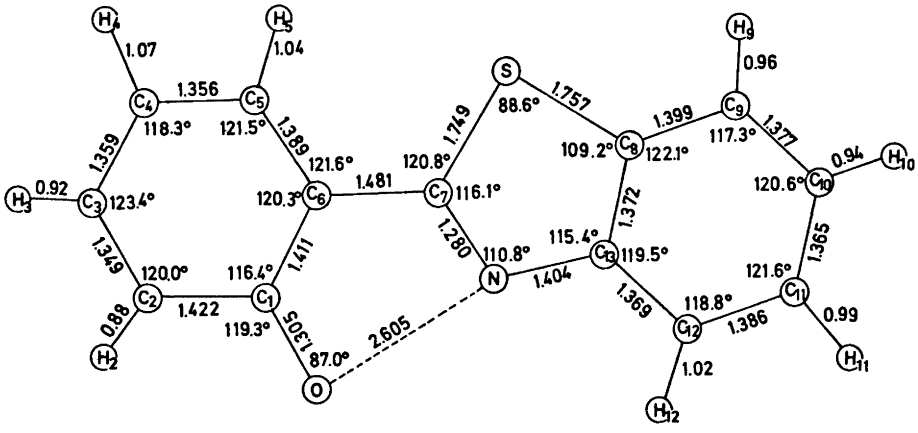


Fig. 1. Schematic drawing of one molecule of 2-(*o*-hydroxyphenyl)benzothiazole showing interatomic distances (Å) and angles (°).

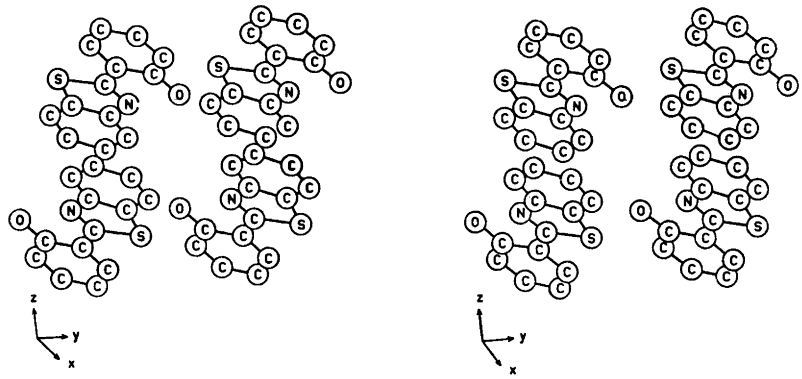


Fig. 2. A stereoscopic pair of drawings of the structure of 2-(*o*-hydroxyphenyl)benzothiazole.

Table 5. A comparison between selected interatomic distances (Å) and angles (°) in structures of benzothiazoles and benzothiazolines, determined by X-ray diffraction methods. Available standard deviations are included.
1 = 2-(*o*-hydroxyphenyl)benzothiazole (this paper).
2 = 1,4-bis-(*N*-ethyl-1,2-dihydrobenzothiazole-2-ylidene)tetrazene.[6]
3*a* and 3*b* = two different benzothiazole groups in bis(*N*-ethyl-2-benzothiazolyl)phosphamethinecyanine perchlorate.[7]
4 = 3-methylbenzothiazoline-2-thione.[8]
5 = [2-(1-methylquinoline)][2-(3-methylbenzothiazole)] methylmonomethincyanine iodide.[9]
6 = benzothiazoline-2-thione.[10]

	1	2	3*a*	3*b*	4	5	6
C_8-C_9	1.399 (12)	1.396 (5)	1.40	1.37	1.38	1.39	1.35
C_9-C_{10}	1.377 (12)	1.382 (6)	1.40	1.43	1.36	1.39	1.35
$C_{10}-C_{11}$	1.365 (12)	1.406 (6)	1.37	1.37	1.41	1.51	1.41
$C_{11}-C_{12}$	1.386 (11)	1.379 (5)	1.41	1.43	1.38	1.43	1.34
$C_{12}-C_{13}$	1.369 (11)	1.398 (5)	1.44	1.40	1.36	1.37	1.34
$C_{13}-C_8$	1.372 (10)	1.405 (4)	1.36	1.37	1.41	1.46	1.42
$N-C_{13}$	1.404 (9)	1.390 (4)	1.38	1.40	1.45	1.35	1.39
$N-C_7$	1.278 (9)	1.371 (4)	1.37	1.34	1.43	1.61	1.29
$S-C_7$	1.750 (7)	1.759 (3)	1.73	1.75	1.77	1.73	1.75
$S-C_8$	1.758 (7)	1.759 (3)	1.744	1.737	1.78	2.09	1.75
$C_8-C_9-C_{10}$	117.0 (7)	118.6 (4)	116	118	115	117	114
$C_9-C_{10}-C_{11}$	120.8 (7)	120.9 (4)	122	121	123	120	124
$C_{10}-C_{11}-C_{12}$	121.4 (7)	120.6 (4)	123	121	122	120	123
$C_{11}-C_{12}-C_{13}$	118.8 (7)	119.3 (3)	115	116	116	121	114
$C_{12}-C_{13}-C_8$	119.6 (7)	119.9 (3)	122	121	122	117	124
$C_{13}-C_8-C_9$	122.4 (7)	120.9 (3)	123	123	122	126	121
$C_8-C_{13}-N$	115.4 (6)	112.2 (3)	114	114	115	115	123
$C_{13}-N-C_7$	110.9 (6)	115.1 (3)	114	113	113	161	95
$N-C_7-S$	116.1 (6)	110.9 (3)	109	111	109	113	129
C_7-S-C_8	88.5 (3)	90.6 (2)	92.4	91.5	94	88	83
$S-C_8-C_{13}$	109.1 (5)	111.2 (3)	109	110	109	108	105

The crystal consists of discrete and essentially planar molecules (Fig. 2). The shortest intermolecular distance (hydrogen atoms not included) is 3.37 (1) Å, and is to be found between atoms O and C(5). The forces between separate molecules are thus only of van der Waals type.

It has been shown that in the solid state the chelates of I with Pd [6] and Cu [1] are formed by ring closure through the nitrogen of the heterocyclic ring and the oxygen of the phenyl group. In the pure organic compounds I and II the chelation may occur through a hydrogen bond O–H···N or O–H···X (X = O or S). The present work shows that in compound II the oxygen atom is, as expected, facing the nitrogen and not the sulphur atom. In compound I the chances of finding a hydrogen bond including the chalcogen of the heterocyclic ring are better, and the conditions are at present under investigation.

The interatomic distances and angles (Table 4 and Fig. 1) deviate little from their expected values. Table 5 shows a comparison between crystal structure determinations of compounds containing benzothiazole groups. It may be noticed that the low values of the angles C(8)–C(9)–C(10) and, to a smaller extent, C(11)–C(12)–C(13), which have been observed in the copper chelate of I,[1] persist in the benzothiazoles. The significance of and the reason for this effect are not yet established and will be examined further in other members of the group of compounds under investigation.

Hydrogen atoms. In the refinement of the atomic positions approximate coordinates for the nine hydrogen atoms were introduced. The refinement resulted in reasonable values for eight hydrogen atoms, and they have been included in Tables 2–4. The position of the hydrogen belonging to the hydroxyl group could not be found. It is quite obvious, though, that there is an intramolecular hydrogen bond between the oxygen and nitrogen atoms. The distance O–N is 2.605(9) Å, which indicates a strong hydrogen bond, and IR measurements using the potassium bromide technique confirm this fact. There is no sharp OH absorption band but a very broad absorption at 2700–3000 cm^{-1}, found in many other compounds containing intramolecular chelating hydrogen bonds. Furthermore, the presence of an intramolecular hydrogen bond and no intermolecular hydrogen bonds is manifested in the low melting point of 129°C for 2-(*o*-hydroxyphenyl)benzothiazole (II), as compared to 229°C for 2-(*p*-hydroxyphenyl)benzothiazole, a compound which could not possibly have any intramolecular hydrogen bonds.

Finally, the planarity of the molecule was investigated using the program PLANE. The best fitting plane has been defined by the positions of the atoms

Table 6. Deviations (Å) from the best fitting plane for one molecule of 2-(*o*-hydroxyphenyl)benzothiazole.

O	0.038	C(7)	0.011	H(2)	−0.147
C(1)	0.002	S	0.050	H(3)	−0.033
C(2)	0.028	N	−0.010	H(4)	0.034
C(3)	−0.004	C(8)	0.009	H(5)	−0.094
C(4)	−0.048	C(13)	−0.029	H(9)	−0.149
C(5)	−0.021	C(9)	0.014	H(10)	0.033
C(6)	0.005	C(10)	0.004	H(11)	−0.024
		C(11)	−0.002	H(12)	−0.007
		C(12)	−0.043		

other than hydrogen. Table 6 shows the result, including distances from the calculated plane to the hydrogen atoms. The molecule is fairly planar, more so than the corresponding molecule in the previously described copper chelate of I.[1]

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