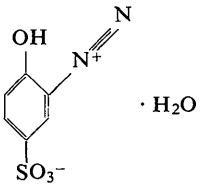
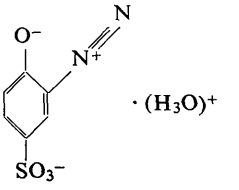
conclusion directly by the neutron diffraction method.

This rather fully developed system of hydrogen bonds together with the ionic interaction between positive diazonium nitrogen atoms and sulfonate oxygen atoms in all probability provides the necessary minimization of the energy to make the diazonium form so stable. Also the zwitterion character of the molecule and the electrostatic attraction in the crystal structure account for the infeasibility of preparing alkaline salts of the compound.



(*a*) 2-Diazonium-4-phenolsulfonate monohydrate



(*b*) The less likely hydronium 2-diazonium-4-sulfophenolate

Fig. 8. Possible chemical formulas.

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Crystal and Molecular Structure of 3-Hydroxy-5-phenylisoxazole (β form)

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The crystal structure of the β form of 3-hydroxy-5-phenylisoxazole has been determined from three-dimensional X-ray data. The crystals, which are obtained either by sublimation or by slowly cooling the melt in the atmosphere, are monoclinic, space group $P2_1/c$, with four molecules in the unit cell. The cell dimensions are: $a=8{\cdot}75$, $b=5{\cdot}64$, $c=16{\cdot}10$ Å, $\beta=95{\cdot}9°$. The structure was refined by the block-diagonal least-squares method to a final R value of 0·084 for 1116 observed reflexions. The molecule is present in the hydroxyl form and the values of bond distances suggest a conjugation effect between isoxazole and benzene rings. Pairs of molecules form dimers linked together by two hydrogen bonds across a centre of symmetry.

Introduction

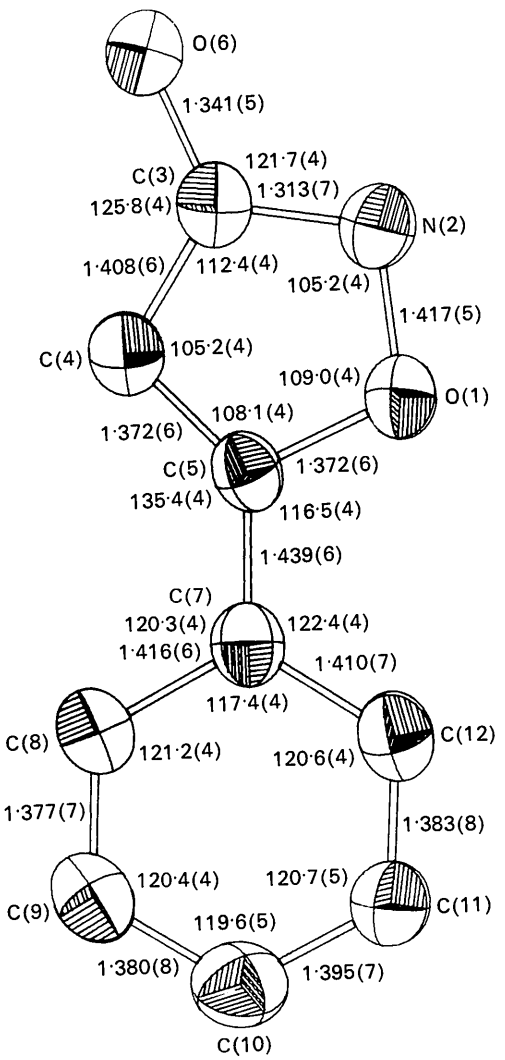
In the course of the investigation of the crystal structure of 3-hydroxy-5-phenylisoxazole (Fig. 1), two crystalline forms were identified. One (α) is obtained when an n-hexane solution is allowed to crystallize; the crystals are colourless prisms, space group $P2_1/c$. The crystal structure has already been reported in a short communication (Cannas & Mocci, 1965) and the refinement, based on three-dimensional data, is now being completed. A second type of crystallization (β) was detected during the determination of the melting point of the α form with a hot stage microscope. It was noticed that at a temperature around 140 °C the compound sublimes

and forms needle-shaped crystals. The analysis of the Debye spectra confirmed the presence of two crystallographic forms.

The investigation of the crystal structure of the β form of 3-hydroxy-5-phenylisoxazole was undertaken to make possible a comparison of the two polymorphic forms.

Experimental

3-Hydroxy-5-phenylisoxazole was prepared by the method of Bravo, Gaudiano, Quilico & Ricca (1961). Crystals of the β form suitable for X-ray analysis were obtained by slowly cooling the melt in the atmosphere.



Fig, 1. Molecular diagram representing the principal axes of the thermal ellipsoids, bond lengths (Å) and angles (°). The diagram was produced with the program of Johnson (1965); bond lengths and angles were calculated by the *X-Ray* 63 *Bondla* program (Stewart *et al.*, 1964), which takes account of the standard deviations of both the lattice constants and the atomic parameters.

The unit-cell dimensions were determined from zero level Weissenberg photographs around [100] and [010]. Their values, compared with those of the α form, are as follows:

3-Hydroxy-5-phenylisoxazole (C_9H_7NO), M.W. 161·66, m.p. 163–64°.

β form	α form
$a = 8{\cdot}75 \pm 0{\cdot}02$ Å	$a = 10{\cdot}42 \pm 0{\cdot}02$ Å
$b = 5{\cdot}64 \pm 0{\cdot}02$	$b = 3{\cdot}89 \pm 0{\cdot}02$
$c = 16{\cdot}10 \pm 0{\cdot}04$	$c = 20{\cdot}82 \pm 0{\cdot}04$
$\beta = 95{\cdot}9 \pm 0{\cdot}2°$.	$\beta = 113{\cdot}6° \pm 0{\cdot}2°$.
D_c ($Z=4$) 1·35 g.cm^{-3}	D_c ($Z=4$) 1·38 g.cm^{-3}
Space group $P2_1/c$	Space group $P2_1/c$

Two crystals, with approximate cross section 0·3 × 0·3 mm, were used for the X-ray analysis, one mounted along the a axis and the other along the b axis. Integrated equi-inclination Weissenberg photographs were taken on multiple films for the layers $0 \le h \le 3$ and $0 \le k \le 4$, using Ni-filtered Cu $K\alpha$ radiation. Of the 1591 independent reflexions recorded, 1131 were in the observable range and their relative intensities were determined photometrically with the aid of a microdensitometer. Intensities were converted to observed structure factors in the usual way. No correction for absorption was made. A standard deviation for each intensity was estimated in the following manner. The reflexions were divided into five intensity ranges: within four of these a constant fractional error was assumed and, with this assumption, the standard deviation is given by $\sigma^2 = KI$, where $K = 1; 0{\cdot}5; 0{\cdot}3; 0{\cdot}1$ respectively. The reflexions which appeared in the fifth range were too weak to be estimated with any accuracy and they were excluded from the rescaling and refinement procedures. The data were placed on the same relative scale by the least-squares procedure of Rae (1965). The atomic scattering factors were interpolated from the values given in *International Tables for X-ray Crystallography* (1962).

Structure solution and refinement

The Patterson projection along the unique axis showed a similar distribution of peaks in the two polymorphs, if the relative orientations of the a and c axes were properly chosen. In this situation the relationship of the indices of the planes in the two forms is

$$h_\alpha = -h_\beta - \tfrac{1}{2} l_\beta ,$$
$$l_\alpha = \; l_\beta .$$

An electron density projection, evaluated by assigning to a set of low θ $F_{o\beta}$ the signs of the pertinent $F_{o\alpha}$, gave the structure which was refined with four successive Fourier synthesis to an R value of 0·22 for the observed $h0l$ reflexions.

The y coordinates were then estimated from the projected distances by a comparison with the expected

values and three-dimensional refinement was carried out by the block-diagonal least-squares method, using the programs I.C.R. No. 4 (van der Helm, 1962) and I.C.R No. 7 (Johnson & Glusker, 1966). The minimized quantity is $\Sigma w(kF_o-F_c)^2$. The weights were given values equal to $1/\sigma^2$. The initial R value was 0·45, which was reduced to 0·14 with twelve cycles of isotropic refinement based on heavy atoms. In the last two cycles the hydrogen atoms of the benzene ring were introduced at the expected positions and were assigned isotropic temperature factors, with $B=4{\cdot}5$ Å^2. Neither the positional parameters nor the temperature factors for the hydrogen atoms were allowed to vary throughout the subsequent least-squares cycles, though their contributions to the structure factors were always incorporated.

Final refinement was carried out by assigning to the heavy atoms anisotropic temperature factors of the form

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

15 of the strongest reflexions, which were suspected of suffering from secondary extinction or from particularly bad measurements were given zero weight. After six cycles no atom parameter shifted as much as one half of its standard deviation. A difference map was computed at this point and all the hydrogen atom positions were readily found; no attempt has been made to refine their parameters. The final R value for 1116 observed reflexions is 0·084. The final positional and thermal parameters and their standard deviations are listed in Table 1. The observed and calculated structure factors are shown in Table 2.

Discussion

In contrast to the isomeric 3-phenylisoxazolin-5-one previously reported (Cannas, Biagini & Marongiu, 1969), 3-hydroxy-5-phenylisoxazole exists in the hydroxyl form in both polymorphs. Bravo *et al.* (1961) proposed this form after infrared and ultraviolet studies of the solution.

The bond distances and angles involving the heavy atoms are given in Fig. 1, and those involving the hydrogen atoms are given in Table 3.

The geometry of the benzene ring is not significantly different from the expected hexagonal symmetry, with an average C–C distance of 1·393 Å. Bond lengths and angles in the isoxazole ring can be compared with those found in 5-5′-biisoxazole (Cannas & Marongiu, 1968), because in both molecules the inter-ring bond is through C(5). It is found that the possibly significant differences in the ring parameters are those involving the C(5) atom: C(4)–C(5) bond lengths are 1·323 Å in

Table 1. *Final positional and thermal parameters*

The estimated standard deviations given in parentheses refer to the last decimal position.

	X	Y	Z	B_1	B_2	B_3
O(6)	0·1669 (4)	0·1157 (5)	0·5821 (2)	4·42	5·88	9·63
O(1)	0·0944 (3)	0·3832 (5)	0·3883 (2)	3·83	5·82	7·11
N(2)	0·0627 (4)	0·2096 (6)	0·4479 (2)	3·96	5·87	6·06
C(3)	0·1609 (5)	0·2518 (8)	0·5135 (2)	4·33	4·98	5·79
C(4)	0·2597 (4)	0·4427 (7)	0·5006 (2)	4·39	5·85	6·05
C(5)	0·2132 (4)	0·5239 (7)	0·4217 (2)	3·59	4·15	5·73
C(7)	0·2618 (4)	0·7096 (7)	0·3689 (2)	3·82	4·73	5·92
C(8)	0·3846 (5)	0·8616 (7)	0·3980 (2)	4·46	5·62	6·37
C(9)	0·4312 (5)	1·0431 (8)	0·3491 (3)	4·67	6·16	7·50
C(10)	0·3563 (5)	1·0843 (9)	0·2708 (3)	5·09	6·92	7·67
C(11)	0·2350 (5)	0·9372 (9)	0·2403 (3)	4·64	5·88	9·27
C(12)	0·1873 (5)	0·7546 (9)	0·2886 (3)	4·39	6·64	7·86
H(6)	0·074	−0·018	0·574			
H(4)	0·345	0·546	0·541			
H(8)	0·428	0·814	0·455			
H(9)	0·534	1·150	0·373			
H(10)	0·395	1·196	0·234			
H(11)	0·188	0·960	0·179			
H(12)	0·090	0·620	0·265			

	11	22	33	12	13	23
O(6)	0·02390 (56)	0·05499 (133)	0·00534 (14)	−0·01493 (152)	−0·00437 (43)	0·00417 (69)
O(1)	0·01582 (39)	0·04828 (119)	0·00541 (13)	−0·00542 (122)	−0·00310 (36)	0·00153 (63)
N(2)	0·01500 (48)	0·04562 (146)	0·00526 (15)	−0·00430 (147)	−0·00116 (43)	0·00209 (76)
C(3)	0·01605 (56)	0·04120 (162)	0·00476 (17)	0·00104 (165)	−0·00015 (48)	−0·00244 (84)
C(4)	0·01663 (59)	0·04624 (186)	0·00510 (19)	−0·00397 (172)	−0·00058 (52)	−0·00130 (90)
C(5)	0·01208 (48)	0·03426 (156)	0·00524 (17)	0·00084 (151)	0·00005 (44)	−0·00282 (80)
C(7)	0·01293 (47)	0·04255 (166)	0·00495 (17)	0·00356 (147)	0·00056 (46)	−0·00277 (83)
C(8)	0·01663 (60)	0·04293 (177)	0·00574 (19)	−0·00474 (185)	0·00059 (55)	−0·00360 (95)
C(9)	0·01839 (72)	0·04781 (200)	0·00652 (23)	−0·00996 (194)	0·00214 (63)	−0·00523 (105)
C(10)	0·01993 (82)	0·05710 (226)	0·00642 (24)	−0·00009 (209)	0·00597 (73)	0·00277 (117)
C(11)	0·01817 (67)	0·06032 (220)	0·00618 (22)	−0·00882 (203)	−0·00266 (60)	0·00754 (110)
C(12)	0·01721 (66)	0·05789 (197)	0·00597 (20)	−0·01040 (202)	−0·00150 (60)	−0·00058 (108)

5,5′-biisoxazole and 1·372 Å in 3-hydroxy-5-phenylisoxazole (β form); the C(5)–O(1) bond lengths are 1·343 and 1·372 Å and the inter-ring bond lengths 1·483 and 1·439 Å respectively. These differences might be attributed to the difference in the conjugation effect between the rings in the two molecules, which should be greater in 3-hydroxy-5-phenylisoxazole (β form).

The interaction between isoxazole and benzene rings has been investigated in phenylisoxazoles by Pino & Speroni (1955) and by Del Re (1962). They concluded that interaction takes place in the case of 5-phenylisoxazole as a result of the combination of the presence of a diene chain connected head to tail to the phenyl group and to the low aromaticity of isoxazole.

Table 2. *Observed and calculated structure factors*

Columns are: h, l, $10F_{obs}$, $10F_{calc}$. Unobserved reflexions are marked with an asterisk and have been given values corresponding to half the estimated minimum observable intensity. Reflexions marked with two asterisks are apparently affected by extinction.

h	l	10Fobs	10Fcalc
K=0			
1	0	285 **	346
2	0	506 **	-643
3	0	318 **	-366
4	0	102	-116
5	0	141	144
6	0	137	-153
7	0	82	-84
8	0	9	-7
9	0	35	-35
10	0	18	-22
11	0	27	23
0	2	255 **	314
1	2	802 **	1035
-1	2	164	-187
2	2	81	-76
-2	2	164	183
3	2	147	158
-3	2	358 **	-415
4	2	104	106
-4	2	112	-118
5	2	147	152
-5	2	286	-301
6	2	35	33
-6	2	77	-87
7	2	76	-84
-7	2	132	140
8	2	65	-67
-8	2	28	29
9	2	74	-78
-9	2	23	-20
10	2	26	-22
-10	2	6 *	1
0	4	39	-34
1	4	64	-62
-1	4	159	180
2	4	277	-289
-2	4	292	-333
3	4	119	119
-3	4	47	-41
4	4	301	344
-4	4	112	-115
5	4	231	251
-5	4	106	-124
6	4	164	180
-6	4	45	37
7	4	85	-87
-7	4	43	40
8	4	54	-58
-8	4	48	52
9	4	27	-27
-9	4	8 *	0
10	4	28	-25
-10	4	46	-42
-11	4	20	-22
0	6	423	-436
1	6	316	-349
-1	6	32	-32
2	6	113	111
-2	6	40	40
3	6	33	36
-3	6	31	26
4	6	116	113
-4	6	110	106
5	6	88	-102
-5	6	34	-35
6	6	84	90
-6	6	104	-105
7	6	218	231
-7	6	39	37
8	6	14	-6
-8	6	18	21
9	6	46	-39
-9	6	7 *	-7
10	6	28	-25
-10	6	29	-26
0	8	229	241
-1	8	5 *	10
2	8	130	-134
-2	8	142	-148
3	8	35	24
-3	8	79	75
4	8	13	13
-4	8	29	33
5	8	21	17
-5	8	173	-188
6	8	144	-149
-6	8	8 *	-3
7	8	55	58
-7	8	31	32
8	8	130	112
-8	8	41	40
9	8	15	15
-9	8	19	-10
-10	8	37	-33
0	10	95	95
1	10	167	166
-1	10	39	-47
2	10	69	-66
-2	10	123	-131
3	10	37	-31
-3	10	140	-148
4	10	44	-41
-4	10	116	-123
5	10	20	-20
-5	10	52	57
6	10	12	14
-6	10	62	60
7	10	3 *	0
-7	10	25	25
8	10	32	30
-8	10	16	21
9	10	21	-15
-9	10	31	-29
-10	10	43	40
0	12	65	59
1	12	59	-62
-1	12	17	22
2	12	96	-96
-2	12	94	-97
3	12	52	-53
-3	12	72	-72
4	12	47	43
-4	12	15	-10
5	12	56	57
-5	12	57	56
6	12	22	23
-6	12	22	22
7	12	40	-27
-7	12	46	46
8	12	7	-7
-8	12	20	14
-9	12	19	18
0	14	57	62
1	14	70	-80
-1	14	61	63
2	14	184	-188
-2	14	28	33
3	14	53	-42
-3	14	63	-64
4	14	47	40
-4	14	59	54
5	14	35	27
-5	14	51	52
6	14	42	33
-6	14	8 *	-6
7	14	17	14
-7	14	17	16
-8	14	7 *	13
0	16	16	14
1	16	8 *	6
-1	16	46	48
2	16	64	-64
-2	16	8 *	3
3	16	78	-63
-3	16	80	78
4	16	16	14
-4	16	64	71
5	16	9	5
-5	16	77	-66
6	16	27	-21
-6	16	26	-22
0	18	20	15
1	18	13	-11
-1	18	33	26
2	18	14	12
-2	18	37	35
3	18	11	9
-3	18	44	43
4	18	15	8
-4	18	41	-40
-5	18	21	-19
-6	18	3 *	-5
0	20	4 *	5
1	20	3 *	3
-1	20	4 *	-5
-2	20	4 *	5
-3	20	4 *	-3
K=1			
1	0	85	-88
2	0	346 **	-434
3	0	339 **	-423
4	0	143	-145
5	0	83	74
6	0	41	36
7	0	54	-51
8	0	3 *	-0
9	0	9	14
10	0	3 *	5
11	0	19	23
0	1	78	81
1	1	47	38
-1	1	291 **	348
2	1	142	133
-2	1	569 **	-773
3	1	23	-21
-3	1	88	61
4	1	222	233
-4	1	129	127
5	1	103	-100
-5	1	76	-73
6	1	138	-131
-6	1	48	-45
7	1	37	-35
-7	1	56	-54
8	1	25	24
-8	1	38	39
9	1	5 *	7
-9	1	51	54
10	1	*	4
-10	1	20	17
0	2	194	-210
1	2	252	-274
-1	2	466 **	635
2	2	143	-154
-2	2	704 **	995
3	2	156	151
-3	2	46	54
4	2	14	9
-4	2	120	-116
5	2	177	-174
-5	2	119	-119
6	2	85	-85
-6	2	44	-51
7	2	98	-102
-7	2	3 *	-4
8	2	65	-67
-8	2	8 *	9
9	2	47	44
-9	2	22	25
10	2	34	33
-10	2	21	-16
0	3	212	225
1	3	228	232
-1	3	639 **	-892
2	3	252	282
-2	3	329 **	-394
3	3	108	-104
-3	3	167	221
4	3	35	-38
-4	3	108	106
5	3	62	61
-5	3	72	76
6	3	31	31
-6	3	80	-71
7	3	28	26
-7	3	47	45
8	3	55	-54
-8	3	68	70
9	3	3 *	-6
-9	3	3 *	1
10	3	2 *	-1
-10	3	20	-24
0	4	22	25
1	4	87	79
-1	4	342 **	423
2	4	323	342
-2	4	125	-126
3	4	153	157
-3	4	32	-25
4	4	46	42
-4	4	98	96
5	4	74	-80
-5	4	77	-74
6	4	75	-76
-6	4	40	-41
7	4	33	-36
-7	4	66	-69
8	4	91	-94
-8	4	15	13
9	4	57	-51
-9	4	36	37
10	4	23	24
-10	4	23	-23
0	5	87	80
1	5	123	-124
-1	5	40	-37
2	5	85	-82
-2	5	146	-148
3	5	6 *	14
-3	5	55	-62
4	5	123	-119
-4	5	218	223
5	5	47	42
-5	5	47	44
6	5	8	11
-6	5	38	33
7	5	93	97
-7	5	14	17
8	5	43	42
-8	5	3 *	0
9	5	68	-64
-9	5	8	-11
10	5	10	-10
-10	5	28	-31
0	6	30	26
1	6	96	-98
-1	6	32	-35
2	6	95	99
-2	6	92	-95
3	6	294	285
-3	6	145	167
4	6	161	164
-4	6	9	-11
5	6	28	-25
-5	6	26	-20
6	6	81	-80
-6	6	65	-63
7	6	3 *	-2
-7	6	47	-33
8	6	9	11
-8	6	55	54
9	6	35	-34
-9	6	17	-20
10	6	30	-31
-10	6	24	-23
0	7	110	122
1	7	56	55
-1	7	111	127
2	7	279	-263
-2	7	118	125
3	7	61	-57
-3	7	140	152
4	7	62	-70
-4	7	43	-43
5	7	75	-76
-5	7	33	-29
6	7	64	67
-6	7	24	-22
7	7	3 *	5
-7	7	22	18
8	7	34	35
-8	7	26	28
9	7	11	-14
-9	7	76	-66
-10	7	16	-19
0	8	107	104
1	8	24	18
-1	8	3 *	-4
2	8	32	-29
-2	8	53	53
3	8	69	-66
-3	8	7 *	-11
4	8	33	25
-4	8	84	-79
5	8	147	157
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6	9	18	-16
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7	9	9	5
7	9	48	-40
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-10	9	3 *	-2
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6	10	60	-58
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7	10	3 *	-1
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8	10	21	22
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-9	10	3 *	-15
0	11	59	60
1	11	49	-44
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2	11	125	128
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4	11	102	-104
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8	11	2 *	-1
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0	12	117	130
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2	12	10 *	-4
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3	12	28	-27
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6	12	35	-34
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7	12	16	-17
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0	13	73	76
1	13	81	74
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2	13	28	23
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4	13	35	-33
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6	13	3 *	-8
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0	14	6 *	7
1	14	41	39
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3	14	18	20
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-8	14	5 *	-7
0	15	8 *	-11
1	15	4 *	10
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2	15	7 *	-3
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3	15	17	12
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4	15	3 *	8
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5	15	3 *	4
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-6	15	3 *	11
-7	15	15	13
0	16	6 *	-0
1	16	19	20
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2	16	3 *	2
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3	16	6 *	1
-3	16	14	-16
4	16	3 *	-5
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5	16	17	15
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-7	16	17	-12
0	17	5 *	-8
1	17	11	-12
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2	17	14	-18
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3	17	19	-12
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4	17	7	9
-4	17	3 *	-10
-5	17	3 *	3
-6	17	2 *	1
0	18	4 *	-8
1	18	3 *	0
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2	18	3 *	10
-2	18	21	-23
3	18	16	15
-3	18	4 *	5
-4	18	7 *	10
-5	18	6 *	7
0	19	3 *	-4
1	19	28	-24
-1	19	35	36
-2	19	3 *	9
-3	19	3 *	-12
-4	19	3 *	-1
K=3			
1	0	161	-153
2	0	21	14
3	0	6 *	5
4	0	3 *	6
5	0	3 *	1
6	0	48	53
7	0	22	20
8	0	3 *	0
9	0	3 *	10
10	0	13	14
0	1	155	164
1	1	34	-38
-1	1	88	88
2	1	105	-104
-2	1	5 *	-3
3	1	19	-19
-3	1	21	-22
4	1	3 *	5
-4	1	14	-13
5	1	41	39

Table 2 (*cont.*)

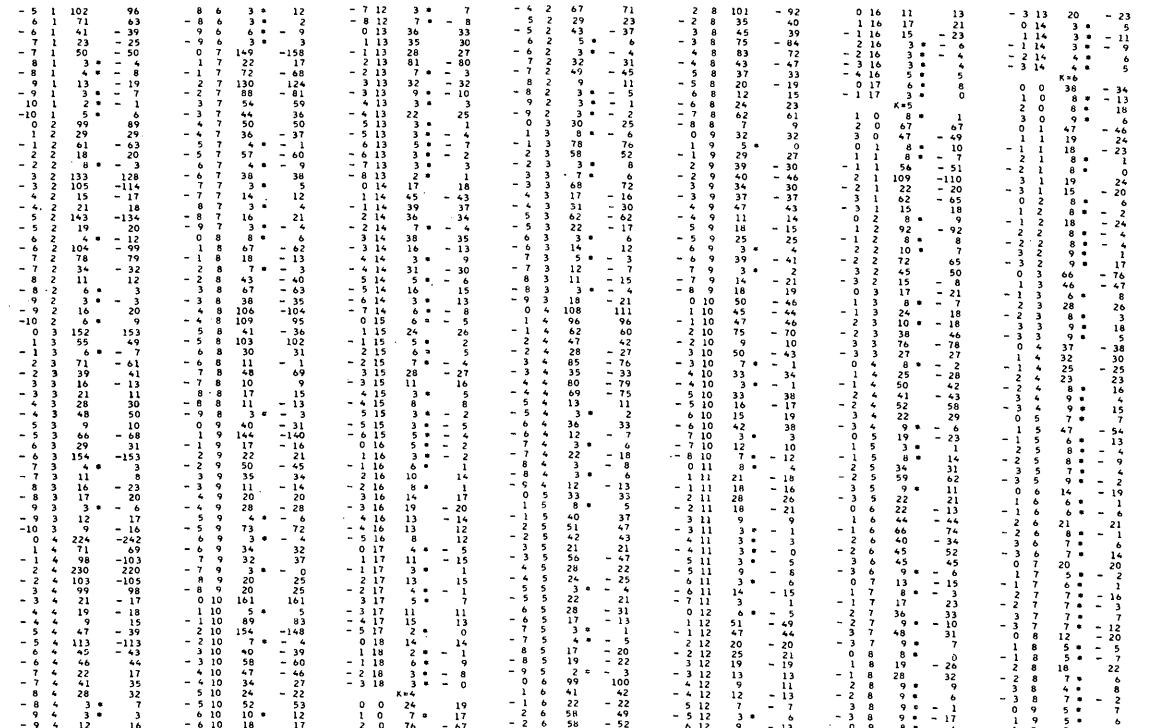

Table 3. *Bond distances and angles involving hydrogen atoms**

O(6)–H(6)	1·13 Å	C(10)–H(10)	0·95 Å
C(4)–H(4)	1·10	C(11)–H(11)	1·04
C(8)–H(8)	0·99	C(12)–H(12)	1·17
C(9)–H(9)	1·15		
C(3)—O(6)–H(6)	106·2°	C(9)—C(10)–H(10)	121·0°
C(3)—C(4)–H(4)	134·6	C(11)–C(10)–H(10)	118·7
C(5)—C(4)–H(4)	119·3	C(10)–C(11)–H(11)	118·7
C(7)—C(8)–H(8)	110·4	C(12)–C(11)–H(11)	120·5
C(9)—C(8)–H(8)	128·4	C(11)–C(12)–H(12)	123·6
C(8)—C(9)–H(9)	120·1	C(7)—C(12)–H(12)	115·6
C(10)–C(9)–H(9)	119·5		

* Because of the lack of accuracy in deriving the hydrogen atom positional parameters from the difference map, the standard deviations in both distances and angles involving hydrogen should be considered to be 0·10 Å and 3° respectively.

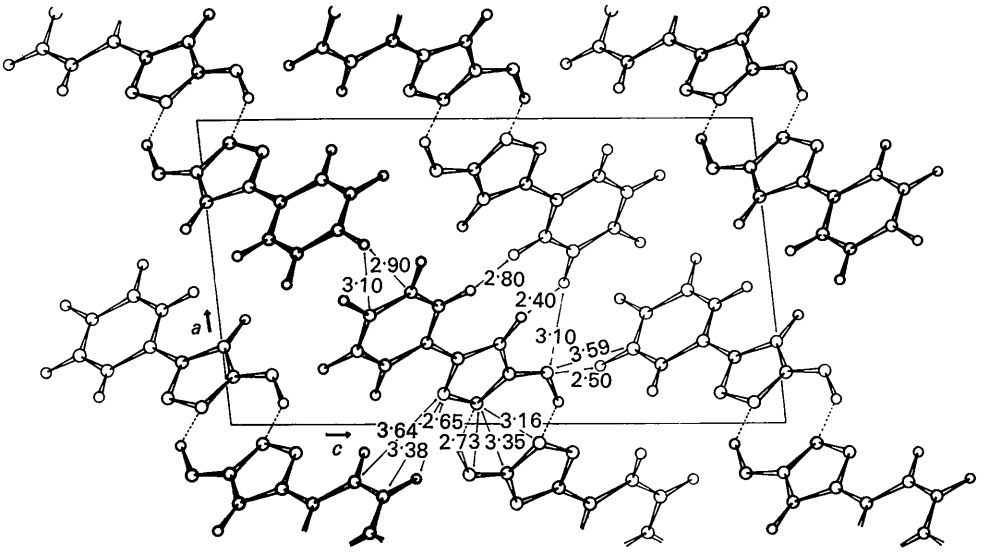

Fig. 2. Projection of the structure along the *b* axis. Dotted lines are intermolecular hydrogen bonds.

The least-squares planes through the entire molecule and the two rings separately were calculated according to the method of Schomaker, Waser, Marsh & Bergman (1959); the results of this analysis are given in Table 4.

Table 4. *Least-squares planes*

Description of planes:

I Complete 3-hydroxy-5-phenylisoxazole molecule
II Isoxazole ring
III Phenyl ring

I $-5{\cdot}997x+3{\cdot}502y+7{\cdot}192z=3{\cdot}587$
II $-6{\cdot}050x+3{\cdot}512y+6{\cdot}979z=3{\cdot}487$
III $-5{\cdot}983x+3{\cdot}471y+7{\cdot}376z=3{\cdot}621$

The equations of the planes are referred to the direct cell. The angle between II and III is 1·6°.

	Distances from planes		
O(6)	−0·0035	0·0273*	−0·0753*
O(1)	0·0188	0·0020	−0·0081*
N(2)	0·0080	0·0040	−0·0348*
C(3)	−0·0227	−0·0082	−0·0776*
C(4)	−0·0059	0·0090	−0·0539*
C(5)	−0·0017	−0·0067	−0·0320*
C(7)	0·0192	0·0036*	0·0037
C(8)	0·0141	0·0094*	−0·0037
C(9)	0·0097	−0·0049*	0·0058
C(10)	−0·0207	−0·0561*	−0·0078
C(11)	−0·0077	−0·0542*	0·0080
C(12)	−0·0076	−0·0446*	−0·0059

* Atoms not included in least-squares plane calculation.

Fig. 2 gives a view of the molecular packing along the *b* axis; all the intermolecular distances between non-hydrogen atoms which are less than 3·7 Å are quoted, whereas for those involving hydrogen atoms, only those less than 3·1 Å are quoted. Pairs of molecules form planar dimers across a centre of symmetry linked together by two hydrogen bonds. The distance O–H...N is 2·726 Å and the O–H...N angle is 174·2°.

The computations in the present analysis were carried out on the IBM 1620 of the Centro di Calcolo of this University.

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