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The Crystal and Molecular Structure of 7-Chloro-1,2-benzoisothiazolin-3-one

BY LUIGI CAVALCA, GIOVANNA FAVA GASPARRI, ALESSANDRO MANGIA AND GIANCARLO PELIZZI
Istituto di Chimica Fisica, Università degli Studi, Parma, Italy

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The crystal structure of 7-chloro-1,2-benzoisothiazolin-3-one has been determined by three-dimensional X-ray analysis. There are four formula units, C_7H_4NOSCl, in the orthorhombic unit cell, $a=23{\cdot}78$ (2), $b=7{\cdot}96$ (2), $c=3{\cdot}859$ (4) Å, space group $P2_12_12_1$. In each molecule the benzene and isothiazole rings are planar and their planes are nearly coincident, the dihedral angle being 179·3°. Steric hindrance between Cl and S is probably responsible for the distortion of the molecule and for the lack of biological activity in the compound. Packing is determined by Cl···Cl van der Waals contacts and by NH···O hydrogen bonds.

Introduction

The investigation of the crystal structure of 7-chloro-1,2-benzoisothiazolin-3-one was undertaken as a part of a programme of study of the molecular structure of a series of antifungal compounds containing the isothiazole ring,* structural information being important in order to correlate the biological activity with the structure of these compounds. Chemical and biological studies (Gialdi, Ponci & Caccialanza, 1964; Ponci, Vitali, Mossini & Amoretti, 1967) have shown that in this series the antifungal activity is strongly reduced when the 7-position is occupied by any substituent and in accordance with this the compound described in the present paper is practically inactive.

A short preliminary account of this structure has already been given (Cavalca, Fava Gasparri, Mangia & Pelizzi, 1968).

* This research is carried out in collaboration with the Istituto di Chimica Farmaceutica della Università di Parma.

Experimental

7-Chloro-1,2-benzoisothiazolin-3-one occurs as very slender colourless orthorhombic needles elongated along [001]. Cell constants, determined from Weissenberg and rotation photographs taken around the elongation axis (Cu $K\alpha$, $\lambda=1{\cdot}5418$ Å), are as follows (standard deviations given in parentheses are in units of the last decimal figure):

C_7H_4NOSCl, $M=185{\cdot}6$; $a=23{\cdot}78$ (2), $b=7{\cdot}96$ (2), $c=3{\cdot}859$ (4) Å; $V=730{\cdot}5$ Å^3, $Z=4$, $D_x=1{\cdot}69$ g.cm^{-3} $\mu=66{\cdot}1$ cm^{-1} (Cu $K\alpha$), $F(000)=376$.

Space group: $P2_12_12_1$ (from systematic absences and structure analysis).

Three-dimensional intensity data were determined photometrically on integrated and non-integrated equi-inclination Weissenberg photographs taken around [001] up to the third layer (multiple-film technique, Cu $K\alpha$); 657 independent reflexions were observed out of a possible 900. By collecting data along the short

axis alone, only 95 independent reflexions (all of the *hk*4 type) remained undetectable.

No absorption correction was used, but the shape of the spots of non-equatorial layers was taken into account following Phillips (1956). After correction for Lorentz and polarization factors, the intensities were placed on the same relative scale with the use of time controlled short oscillation ($\Delta\omega = 20°$) Weissenberg photographs for each layer all registred on the same film; the absolute scale was then established by Wilson's method.

Structure analysis and refinement

The structure was solved by the heavy-atom method, starting from a set of coordinates for the Cl and S atoms deduced from the three-dimensional sharpened Patterson function and refined first by means of two cycles of least-squares with isotropic thermal parameters, then by five cycles of Booth's differential synthesis with anisotropic thermal parameters.

The final residual error indices were (R, for observed reflexions only, R' including $F_o = \frac{1}{2}F_{\min}$ when $F_c \geq F_{\min}$

Table 1. *Final atomic fractional coordinates* ($\times 10^4$), *thermal parameters* ($\times 10$ Å^2)† *with e.s.d.'s and ratios (e.s.d.)/(coordinate shift)*

	$x/a(\sigma)$	$y/b(\sigma)$	$z/c(\sigma)$	$B_{11}(\sigma)$	$B_{22}(\sigma)$	$B_{33}(\sigma)$	$B_{12}(\sigma)$	$B_{13}(\sigma)$	$B_{23}(\sigma)$	$\lvert r(x)\rvert$	$\lvert r(y)\rvert$	$\lvert r(z)\rvert$
Cl	2345 (1)	1885 (3)	714 (7)	30 (1)	35 (1)	40 (1)	1 (2)	3 (1)	−2 (2)	∞	2	7
S	1205 (1)	397 (2)	4397 (6)	30 (1)	24 (1)	32 (1)	2 (1)	2 (1)	0 (1)	∞	2	6
O	−68 (3)	3008 (7)	6603 (18)	30 (3)	26 (2)	40 (3)	0 (4)	5 (4)	−1 (4)	∞	4	5
N	559 (3)	901 (8)	5853 (22)	35 (4)	28 (3)	36 (3)	−5 (5)	3 (5)	−1 (5)	∞	3	11
C(1)	1770 (4)	3177 (9)	1589 (23)	26 (4)	22 (3)	29 (3)	3 (5)	2 (5)	−2 (5)	2	5	23
C(2)	1777 (4)	4844 (10)	705 (25)	37 (4)	31 (3)	32 (3)	−7 (5)	1 (5)	−2 (5)	4	∞	5
C(3)	1304 (4)	5857 (9)	1478 (23)	36 (4)	26 (3)	38 (4)	−3 (6)	1 (6)	3 (6)	2	3	6
C(4)	834 (4)	5189 (10)	3069 (21)	37 (5)	28 (3)	35 (3)	1 (6)	−3 (5)	−3 (5)	4	3	2
C(5)	842 (32)	3485 (9)	3944 (19)	28 (3)	26 (4)	26 (2)	3 (5)	−4 (4)	0 (5)	32	3	2
C(6)	1295 (3)	2451 (10)	3156 (19)	26 (3)	23 (3)	27 (3)	−1 (5)	1 (5)	−1 (5)	2	3	10
C(7)	390 (3)	2502 (8)	5604 (23)	30 (4)	23 (3)	35 (3)	−2 (5)	−1 (5)	−4 (5)	∞	∞	12

† The B_{ij} values refer to the formula $\exp[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)]$ in which $b_{11} = \frac{1}{4}a^{*2}B_{11}$, $b_{12} = \frac{1}{2}a^*b^*B_{12}$, *etc.*

Table 2. *Atomic peak heights* (e.Å^{-3}), *curvatures* (e.Å^{-5}) *and e.s.d.'s*

		ϱ	$-A_{hh}$	$-A_{kk}$	$-A_{ll}$	A_{kl}	A_{hl}	A_{hk}
Cl	obs.	30·0	304	279	218	−5	14	7
	calc.	30·3	301	281	222	−4	11	6
S	obs.	32·2	318	342	243	−1	11	8
	calc.	32·2	318	334	245	−1	8	5
O	obs.	11·7	102	104	78	−4	3	3
	calc.	12·0	102	105	82	−3	2	3
N	obs.	9·9	83	94	66	−2	2	−3
	calc.	9·9	81	92	66	−1	1	−2
C(1)	obs.	8·8	79	86	63	−3	3	5
	calc.	9·2	80	88	64	−2	3	5
C(2)	obs.	7·9	65	71	58	0	1	−3
	calc.	7·9	65	68	58	0	0	−3
C(3)	obs.	8·2	75	77	59	0	−5	−8
	calc.	8·4	77	77	60	0	−5	−7
C(4)	obs.	8·1	66	70	60	−10	−1	2
	calc.	8·2	68	71	60	−9	−1	2
C(5)	obs.	8·9	83	81	66	−5	−4	5
	calc.	9·0	83	80	65	−6	−4	5
C(6)	obs.	8·9	79	71	68	−5	−3	−3
	calc.	8·9	80	71	68	−4	−3	−3
C(7)	obs.	8·8	86	83	60	−5	1	1
	calc.	8·9	84	82	61	−5	2	1
	e.s.d.	0·2	3	3	2	2	2	2

for unobserved reflexions; multiplicities not considered): $R=7{\cdot}5\%$, $R'=10{\cdot}7\%$ and the ratios between the estimated standard deviations and the shifts of the coordinates were as shown in Table 1 in which the final parameters with their e.s.d.'s (Cruickshank, 1949, 1956) are also quoted.

The comparison between observed and calculated peak shapes is shown in Table 2; observed and calculated structure factors are compared in Table 3. The e.s.d.'s for the electron-density first derivatives are: $\sigma(A_h)=0{\cdot}625$, $\sigma(A_k)=0{\cdot}600$, $\sigma(A_l)=0{\cdot}558$ e.Å^{-4}.

Table 3. *Observed and calculated structure factors*

A minus sign for F_o means 'less than'.

h	k	l	$\lvert 10F_o \rvert$	$10F_c$	α'	h	k	l	$\lvert 10F_o \rvert$	$10F_c$	α'	h	k	l	$\lvert 10F_o \rvert$	$10F_c$	α'	h	k	l	$\lvert 10F_o \rvert$	$10F_c$	α'	h	k	l	$\lvert 10F_o \rvert$	$10F_c$	α'
0	1	0	23-	0	0	2	6	1	103	88	135	5	2	0	270	283	270	7	7	2	28-	25	33	10	4	1	261	259	258	13	2	0	61-	48	270
0	1	1	205	179	270	2	6	2	215	206	124	5	2	1	220	236	192	7	7	3	86	86	69	10	4	2	223	209	93	13	2	1	106	108	207
0	1	2	142	135	270	2	6	3	34	38	11	5	2	2	147	130	24	7	8	0	110	98	90	10	4	3	104	106	197	13	2	2	29-	42	16
0	1	3	94	100	90	2	7	0	197	186	180	5	2	3	113	108	242	7	8	1	120	101	158	10	5	0	289	281	180	13	2	3	225	250	255
0	2	0	107	158	180	2	7	1	109	118	284	5	3	0	510	537	270	7	8	2	95	90	130	10	5	1	176	193	157	13	3	0	144	156	270
0	2	1	210	188	180	2	7	2	151	145	150	5	3	1	29-	8	173	7	9	0	58-	87	90	10	5	2	125	103	240	13	3	1	119	106	212
0	2	2	113	116	0	2	7	3	21-	35	36	5	3	2	132	120	274	7	9	1	85	73	33	10	5	3	110	115	191	13	3	2	86	76	253
0	2	3	103	96	180	2	8	0	124	126	0	5	3	3	131	124	71	7	9	2	13-	22	84	10	6	0	77-	125	0	13	3	3	27-	42	6
0	3	0	44-	0	0	2	8	1	41-	16	225	5	4	0	321	315	270	7	10	0	25-	40	90	10	6	1	89	76	126	13	4	0	278	274	270
0	3	1	343	350	270	2	8	2	132	124	60	5	4	1	238	241	330	8	0	0	540	642	0	10	6	2	30-	27	257	13	4	1	41-	54	218
0	3	2	254	244	270	2	8	3	49	66	105	5	4	2	232	228	249	8	0	1	104	73	270	10	6	3	22-	11	10	13	4	2	228	227	240
0	3	3	68	77	270	2	9	0	136	126	180	5	4	3	74	62	183	8	0	2	129	124	0	10	7	0	170	150	180	13	4	3	58	57	266
0	4	0	399	397	0	2	9	1	69	70	72	5	5	0	117	88	90	8	0	3	136	119	270	10	7	1	146	155	258	13	5	0	75-	23	270
0	4	1	33-	9	0	2	9	2	65	53	165	5	5	1	199	192	60	8	1	0	233	266	0	10	7	2	127	137	151	13	5	1	232	238	21
0	4	2	78	59	0	2	10	0	39-	50	180	5	5	2	86	80	131	8	1	1	98	74	52	10	7	3	16-	3	327	13	5	2	79	84	158
0	4	3	27-	31	0	3	0	1	800	909	270	5	5	3	146	144	74	8	1	2	251	243	291	10	8	0	68-	2	0	13	5	3	23-	26	112
0	5	0	62-	0	0	3	0	2	470	452	0	5	6	0	296	290	270	8	1	3	178	183	53	10	8	1	36-	61	281	13	6	0	77-	33	270
0	5	1	352	353	270	3	0	3	267	279	270	5	6	1	240	236	171	8	2	0	202	177	180	10	8	2	66	63	74	13	6	1	61	61	121
0	5	2	33	34	270	3	1	0	29-	23	90	5	6	2	75	59	331	8	2	1	479	526	144	10	9	0	125	107	180	13	6	2	66	62	197
0	5	3	28	35	270	3	1	1	454	447	16	5	6	3	53	53	150	8	2	2	169	156	17	10	9	1	45	45	30	13	6	3	55	50	15?
0	6	0	119	129	0	3	1	2	286	254	129	5	7	0	100	117	270	8	2	3	226	226	170	11	0	1	111	112	270	13	7	0	73-	55	270
0	6	1	217	217	180	3	1	3	156	144	94	5	7	1	147	139	191	8	3	0	53-	29	0	11	0	2	279	280	0	13	7	1	40-	56	218
0	6	2	52	41	0	3	2	0	291	277	270	5	7	2	146	137	182	8	3	1	217	226	235	11	0	3	52	64	270	13	7	2	127	131	179
0	6	3	153	172	180	3	2	1	408	412	26	5	7	3	36	45	315	8	3	2	162	146	274	11	1	0	261	267	90	13	7	3	7-	11	128
0	7	0	77-	0	0	3	2	2	90	74	218	5	8	0	79	72	270	8	3	3	105	100	264	11	1	1	138	121	0	13	8	0	61-	59	270
0	7	1	43-	81	90	3	2	3	124	120	311	5	8	1	125	127	193	8	4	0	221	198	0	11	1	2	131	99	68	13	8	1	33-	23	127
0	7	2	45	52	90	3	3	0	574	561	90	5	8	2	70	67	300	8	4	1	74	86	351	11	1	3	71	70	130	13	8	2	73	74	279
0	7	3	77	71	270	3	3	1	214	209	14	5	8	3	10-	3	109	8	4	2	195	187	283	11	2	0	642	662	270	13	9	0	40-	18	90
0	8	0	114	157	180	3	3	2	318	313	101	5	9	0	61-	29	90	8	4	3	52	51	186	11	2	1	244	238	47	14	0	0	128	136	180
0	8	1	41-	2	180	3	3	3	197	193	317	5	9	1	84	91	121	8	5	0	171	154	180	11	2	2	133	116	282	14	0	1	488	508	90
0	8	2	80	61	180	3	4	0	55-	6	270	5	9	2	47	32	103	8	5	1	261	266	283	11	2	3	27-	36	3	14	0	2	148	162	180
0	8	3	13-	38	180	3	4	1	169	128	272	5	10	0	34-	67	270	8	5	2	112	101	105	11	3	0	258	265	90	14	0	3	95	90	90
0	9	0	63-	0	0	3	4	2	120	118	347	6	0	0	312	351	180	8	5	3	93	81	352	11	3	1	184	171	340	14	1	0	61-	76	180
0	9	1	128	142	270	3	4	3	80	73	275	6	0	1	398	441	90	8	6	0	75-	11	180	11	3	2	131	149	110	14	1	1	128	107	305
0	9	2	17-	15	90	3	5	0	221	212	270	6	0	2	205	205	180	8	6	1	176	172	161	11	3	3	130	131	285	14	1	2	150	141	135
0	10	0	40-	8	180	3	5	1	151	137	348	6	0	3	47	43	90	8	6	2	106	97	341	11	4	0	195	218	90	14	1	3	119	108	71
0	10	1	17-	29	180	3	5	2	198	188	201	6	1	0	318	334	180	8	6	3	138	145	191	11	4	1	39-	35	255	14	2	0	63-	53	180
1	0	1	350	321	90	3	5	3	63	72	235	6	1	1	275	257	302	8	7	0	182	153	0	11	4	2	87	81	337	14	2	1	39-	64	207
1	0	2	240	221	180	3	6	0	235	222	270	6	1	2	353	338	241	8	7	1	153	145	240	11	4	3	55	56	346	14	2	2	132	134	260
1	0	3	90	87	90	3	6	1	281	284	55	6	1	3	163	166	357	8	7	2	113	111	27	11	5	0	136	125	90	14	2	3	102	106	65
1	1	0	110	134	90	3	6	2	237	216	339	6	2	0	83	83	180	8	7	3	52	41	222	11	5	1	198	211	214	14	3	0	144	160	0
1	1	1	567	598	225	3	6	3	26-	30	324	6	2	1	157	147	88	8	8	0	151	149	180	11	5	2	140	128	186	14	3	1	120	112	7
1	1	2	273	260	116	3	7	0	77-	47	270	6	2	2	273	264	324	8	8	1	38-	27	77	11	5	3	94	100	254	14	3	2	204	188	27
1	1	3	199	201	244	3	7	1	43-	20	126	6	2	3	165	154	75	8	8	2	97	145	270	11	6	0	215	232	270	14	3	3	122	134	347
1	2	0	202	179	90	3	7	2	29-	51	24	6	3	0	83	65	0	8	9	0	56-	67	180	11	6	1	200	197	18	14	4	0	130	113	180
1	2	1	283	295	114	3	7	3	71	67	308	6	3	1	265	269	67	8	9	1	110	108	263	11	6	2	98	86	289	14	4	1	140	151	64
1	2	2	251	228	30	3	8	0	75-	16	270	6	3	2	357	343	50	8	9	2	10-	12	176	11	6	3	55	63	304	14	4	2	170	164	130
1	2	3	126	122	91	3	8	1	90	68	50	6	3	3	177	177	2	9	0	1	160	176	90	11	7	0	75-	48	90	14	4	3	25-	5	307
1	3	0	184	196	270	3	8	2	94	90	222	6	4	0	84	104	0	9	0	2	123	98	180	11	7	1	41-	21	238	14	5	0	344	343	0
1	3	1	378	371	152	3	8	3	36	28	62	6	4	1	181	189	92	9	0	3	245	266	90	11	7	2	26-	35	150	14	5	1	120	121	54
1	3	2	151	155	332	3	9	0	62-	12	270	6	4	2	65	54	140	9	1	0	513	529	90	11	7	3	41	36	293	14	5	2	96	102	11
1	3	3	59	48	215	3	9	1	85	84	249	6	4	3	84	80	200	9	1	1	106	87	285	11	8	0	66-	8	270	14	5	3	22-	21	159
1	4	0	601	596	90	3	9	2	17-	30	195	6	5	0	252	234	0	9	1	2	109	113	99	11	8	1	117	115	27	14	6	0	77-	47	180
1	4	1	418	426	10	3	10	0	38-	27	270	6	5	1	38-	57	23	9	1	3	25-	60	203	11	8	2	99	88	217	14	6	1	43-	49	142
1	4	2	107	90	29	3	10	1	14-	14	310	6	5	2	211	216	288	9	2	0	242	255	90	11	9	0	48-	45	270	14	6	2	139	131	274
1	4	3	119	117	4	4	0	0	245	294	180	6	5	3	58	61	109	9	2	1	134	103	114	11	9	1	47	43	266	14	6	3	44	38	47
1	5	0	173	186	90	4	0	1	780	871	270	6	6	0	74-	81	180	9	2	2	161	145	54	12	0	0	61	41	180	14	7	0	71-	6	180
1	5	1	79	88	8	4	0	2	72	48	0	6	6	1	216	206	66	9	2	3	37-	34	31	12	0	1	172	160	270	14	7	1	38-	53	324
1	5	2	127	123	71	4	0	3	57	41	90	6	6	2	143	146	261	9	3	0	105	133	270	12	0	2	193	162	180	14	7	2	71	51	83
1	5	3	62	72	191	4	1	0	31-	32	0	6	6	3	83	88	9	9	3	1	382	401	166	12	0	3	99	92	270	14	8	0	60-	3	0
1	6	0	128	112	90	4	1	1	417	415	70	6	7	0	164	131	0	9	3	2	205	205	355	12	1	0	302	307	0	14	8	1	108	106	281
1	6	1	85	84	38	4	1	2	354	298	105	6	7	1	43-	45	263	9	3	3	27-	16	315	12	1	1	234	233	87	14	8	2	13-	81	255
1	6	2	122	117	126	4	1	3	21-	35	80	6	7	2	124	109	9	9	4	0	62-	7	90	12	1	2	213	206	60	15	0	1	92	95	270
1	6	3	86	86	101	4	2	0	860	1000	180	6	7	3	20-	6	260	9	4	1	160	144	2	12	1	3	27-	8	126	15	0	2	133	134	0
1	7	0	153	141	270	4	2	1	95	86	178	6	8	0	73-	36	0	9	4	2	101	90	351	12	2	0	261	252	180	15	0	3	84	89	270
1	7	1	157	143	294	4	2	2	342	329	203	6	8	1	132	129	297	9	4	3	77	82	14	12	2	1	132	124	66	15	1	0	302	291	270
1	7	2	77	69	295	4	2	3	53	45	147	6	8	2	98	95	332	9	5	0	358	354	90	12	2	2	235	231	127	15	1	1	164	166	181
1	7	3	158	170	264	4	3	0	180	183	180	6	9	0	170	168	0	9	5	1	141	156	323	12	3	0	148	85	49	15	1	2	217	208	331
1	8	0	75-	44	90	4	3	1	181	211	97	6	9	1	91	83	97	9	5	2	183	176	9	12	3	1	144	153	180	15	1	3	27-	30	226
1	8	1	116	104	13	4	3	2	24-	45	121	6	9	2	51	37	18	9	5	3	40	48	190	12	3	2	195	199	147	15	2	0	67-	50	270
1	8	2	80	87	13	4	3	3	160	150	174	6	10	0	31-	17	0	9	6	0	275	259	90	12	3	3	74	75	115	15	2	1	205	189	153
1	9	0	63-	66	270	4	4	0	181	148	180	7	0	1	94	97	270	9	6	1	79	83	258	12	3	3	117	113	174	15	2	2	131	120	199
1	9	1	35-	30	345	4	4	1	405	406	353	7	0	2	259	251	180	9	6	2	161	159	102	12	4	0	130	117	180	15	2	3	73	84	101
1	9	2	77	83	326	4	4	2	27-	28	158	7	0	3	23-	7	90	9	6	3	23-	21	345	12	4	1	140	107	343	15	3	0	117	166	270
1	10	0	40-	41	90	4	4	3	243	257	355	7	1	0	269	418	270	9	7	0	77-	22	90	12	4	2	71	87	195	15	3	1	116	104	12
2	0	0	19-	23	0	4	5	0	64-	61	180	7	1	1	338	347	155	9	7	1	43-	62	240	12	4	3	108	120	347	15	3	2	61	47	176
2	0	1	433	489	270	4	5	1	148	127	95	7	1	2	266	269	296	9	7	2	27-	26	232	12	5	0	133	104	180	15	3	3	45	59	50
2	0	2	216	166	180	4	5	2	102	80	130	7	1	3	186	191	91	9	7	3	20-	27	261	12	5	1	310	301	60	15	4	0	318	337	90
2	0	3	39	52	270	4	5	3	41	32	166	7	2	0	148	132	270	9	8	0	162	158	90	12	5	2	83	80	175	15	4	1	180	159	167
2	1	0	750	833	180	4	6	0	144	135	0	7	2	1	305	300	28	9	8	1	58	64	7	12	5	3	90	99	4	15	4	2	145	130	117
2	1	1	772	883	288	4	6	1	42-	54	251	7	2	2	228	206	182	9	8	2	67	66	89	12	6	0	299	301	0	15	4	3	51	60	159
2	1	2	113	101	154	4	6	2	30-	38	117	7	2	3	207	210	112	9	9	0	54-	52	270	12	6	1	76	72	260	15	5	0	77-	14	90
2	1	3	89	95	157	4	6	3	63	55	48	7	3	0	51-	13	270	9	9	1	28-	46	332	12	6	2	86	87	89	15	5	1	92	100	122
2	2	0	154	136	0	4	7	0	164	193	0	7	3	1	31-	35	297	10	0	0	128	95	180	12	6	3	61	61	341	15	5	2	50	39	353
2	2	1	244	248	283	4	7	1	244	229	88	7	3	2	164	146	322	10	0	1	28-	46	270	12	7	0	75-	4	0	15	5	3	106	102	132
2	2	2	82	84	317	4	7	2	90	76	290	7	3	3	50	47	44	10	0	2	139	143	180	12	7	1	106	93	94	15	6	0	76-	60	270
2	2	3	162	164	338	4	7	3	108	119	104	7	4	0	341	363	90	10	0	3	55	70	270	12	7	2	25-	21	21	15	6	1	156	153	233
2	3	0	45-	25	180	4	8	0	74-	97	180	7	4	1	343	350	224	10	1	0	207	234	180	12	7	3	12-	40	87	15	6	2	45	45	357
2	3	1	191	183	121	4	8	1	40-	32	14	7	4	2	186	163	141	10	1	1	300	205	204	12	8	0	64-	51	180	15	6	3	77	73	233
2	3	2	322	306	136	4	8	2	25-	22	7	7	4	3	42	44	101	10	1	2	217	200	217	12	8	1	70	79	60	15	7	0	69	10	270
2	3	3	122	116	185	4	9	0	61-	44	180	7	5	0	348	374	270	10	1	3	208	223	174	12	8	2	42	32	37	15	7	1	130	110	49
2	4	0	54-	34	0	4	9	1	35-	25	54	7	5	1	159	159	155	10	2	0	194	189	0	12	9	0	103	109	180	15	7	2	66	56	39
2	4	1	140	135	276	4	9	2	39	51	242	7	5	2	227	203	317	10	2	1	331	337	266	12	9	1	46	51	100	15	8	0	55-	16	90
2	4	2	134	106	111	5	0	1	416	441	270	7	5	3	87	83	130	10	2	2	146	139	326	13	0	1	35-	18	270	15	8	1	118	123	144
2	4	3	122	121	163	5	0	2	249	264	180	7	6	0	75-	75	270	10	2	3	167	161	279	13	0	2	66	44	180	15	8	2	7-	21	79
2	5	0	231	232	180	5	0	3	59	49	270	7	6	1	204	189	256	10	3	0	122	117	0	13	0	3	27-	43	90	15	9	0	19	40	90
2	5	1	38-	27	131	5	1	0	221	233	90	7	6	2	58	60	71	10	3	1	96-	68	86	13	1	0	256	262	270	16	0	0	413	426	0
2	5	2	218	219	229	5	1	1	252	264	7	7	6	3	77	76	243	10	3	2	86	99	110	13	1	1	425	445	342	16	0	1	120	127	270
2	5	3	82	80	209	5	1	2	412	417	171	7	7	0	72-	41	90	10	3	3	28-	37	291	13	1	2	179	182	210	16	0	2	30-	58	0
2	6	0	186	210	180	5	1	3	115	108	314	7	7	1	43-	8	209	10	4	0	65-	56	0	13	1	3	90	90	275	16	0	3	27-	31	90

Table 3 (*cont.*)

h	k	l	$10F_o$	$10F_c$	α°	h	k	l	$10F_o$	$10F_c$	α°	h	k	l	$10F_o$	$10F_c$	α°	h	k	l	$10F_o$	$10F_c$	α°	h	k	l	$10F_o$	$10F_c$	α°
16	1	0	381	390	0	17	5	2	164	154	356	19	3	0	77–	44	90	21	1	1	181	188	19	23	0	3	17–	30	270	25	3	1	134	139	158
16	1	1	146	127	331	17	5	3	31	25	291	19	3	1	165	158	9	21	1	2	146	135	195	23	1	0	76–	56	270	25	3	2	103	96	27
16	1	2	206	198	305	17	6	0	108	110	90	19	3	2	69	64	169	21	1	3	43	45	52	23	1	1	91	77	217	25	4	0	56–	21	90
16	1	3	61	68	27	17	6	1	84	78	19	19	3	3	63	67	348	21	2	0	77–	18	90	23	1	2	92	85	321	25	4	1	84	69	176
16	2	0	138	141	0	17	6	2	116	126	88	19	4	0	138	97	90	21	2	1	124	102	329	23	1	3	16–	26	232	25	5	0	47–	50	270
16	2	1	184	172	114	17	7	0	62–	32	270	19	4	1	125	114	344	21	2	2	57	56	164	23	2	0	75–	107	270	25	5	1	22–	37	346
16	2	2	199	202	358	17	7	1	47	44	173	19	4	2	106	99	34	21	2	3	100	114	266	23	2	1	82	68	137	26	0	0	142	127	0
16	2	3	47	46	163	17	8	0	46–	47	90	19	4	3	73	79	16	21	3	0	77–	3	270	23	2	2	69–	76	199	26	0	1	63	57	270
16	3	0	73–	8	180	17	8	1	46	50	308	19	5	0	74–	68	90	21	3	1	43–	25	234	23	2	3	58	73	123	26	0	2	99	92	0
16	3	1	172	164	255	18	0	0	158	124	0	19	5	1	93	84	231	21	3	2	27–	29	116	23	3	0	180	196	270	26	1	0	67–	72	180
16	3	2	30–	36	223	18	0	1	170	157	90	19	5	2	55	51	155	21	3	3	54	58	54	23	3	1	91	77	58	26	1	1	36–	31	98
16	3	3	100	107	206	18	0	2	123	103	0	19	5	3	64	70	260	21	4	0	207	198	270	23	3	2	104	102	277	26	1	2	62	44	180
16	4	0	76–	91	0	18	0	3	26–	48	270	19	6	0	167	140	270	21	4	1	103	78	210	23	4	0	173	177	90	26	2	0	64–	26	180
16	4	1	43–	25	90	18	1	0	210	207	180	19	6	1	113	101	347	21	4	2	117	117	278	23	4	1	36–	32	164	26	2	1	116	112	242
16	4	2	91	70	292	18	1	1	42–	39	121	19	6	2	61	59	219	21	4	3	38	47	225	23	4	2	20–	23	118	26	2	2	77	69	236
16	4	3	37	50	153	18	1	2	112	90	228	19	7	0	55–	33	270	21	5	0	69–	0	0	23	5	0	60–	20	90	26	3	0	50–	12	180
16	5	0	77–	81	0	18	1	3	76	82	182	19	7	1	62	63	274	21	5	1	134	135	349	23	5	1	76	75	150	26	3	1	31–	18	260
16	5	1	164	157	299	18	2	0	74–	41	0	19	8	0	29–	20	90	21	5	2	68	65	220	23	5	2	15–	13	206	26	3	2	81	75	245
16	5	2	92	83	302	18	2	1	277	264	267	20	0	0	315	325	180	21	6	0	59–	52	270	23	6	0	47–	44	270	26	4	0	52–	52	0
16	5	3	80	75	15	18	2	2	91	92	335	20	0	1	166	161	270	21	6	1	30–	29	123	23	6	1	80	94	189	26	4	1	26–	36	314
16	6	0	75–	43	180	18	2	3	64	58	236	20	0	2	107	92	180	21	6	2	14–	36	316	24	0	0	146	146	0	26	5	0	38–	32	180
16	6	1	157	162	252	18	3	0	76–	34	180	20	0	3	45	61	270	21	7	0	43–	19	90	24	0	1	43	39	90	27	0	1	53	64	270
16	6	2	25–	27	350	18	3	1	91	91	261	20	1	0	280	263	0	21	7	1	19–	36	161	24	0	2	25–	12	180	27	0	2	75	80	0
16	6	3	33	56	170	18	3	2	90	81	159	20	1	1	84	71	223	22	0	0	223	202	0	24	0	3	13–	15	270	27	1	0	140	133	90
16	7	0	158	170	0	18	3	3	26	40	336	20	1	2	124	118	60	22	0	1	236	237	90	24	1	0	76–	90	0	27	1	1	47	46	280
16	7	1	70	72	264	18	4	0	77–	17	0	20	1	3	23–	15	169	22	0	2	32	19	180	24	1	1	197	183	203	27	1	2	89	78	97
16	7	2	19–	27	6	18	4	1	43–	61	333	20	2	0	77–	100	180	22	0	3	19–	15	90	24	1	2	85	83	313	27	2	0	107	83	270
16	8	0	108	82	180	18	4	2	138	136	73	20	2	1	43–	65	289	22	1	0	77–	26	0	24	1	3	62	86	0	27	2	1	20	61	119
16	8	1	51	46	87	18	4	3	20–	26	83	20	2	2	107	105	129	22	1	1	57	39	116	24	2	0	73–	84	0	27	2	2	69	68	249
17	0	1	125	112	90	18	5	0	75–	68	180	20	2	3	54	55	8	22	1	2	71	61	140	24	2	1	115	103	97	27	3	0	53–	39	270
17	0	2	122	125	0	18	5	1	96	91	253	20	3	0	230	243	180	22	1	3	45	43	46	24	2	2	75	65	358	27	3	1	27–	24	246
17	0	3	185	203	90	18	5	2	106	90	253	20	3	1	136	138	139	22	2	0	164	174	180	24	3	0	69–	2	180	27	4	0	43	18	90
17	1	0	70–	33	270	18	5	3	54	60	186	20	3	2	90	91	123	22	2	1	70	57	269	24	3	1	37–	46	180	27	4	1	111	125	249
17	1	1	261	255	204	18	6	0	70–	20	0	20	3	3	69	82	165	22	2	2	113	109	242	24	3	2	21–	22	160	28	0	0	148	148	180
17	1	2	188	183	169	18	6	1	86	65	101	24	4	0	76–	107	180	22	2	3	17–	29	66	24	4	0	53–	90	0	28	0	1	103	101	270
17	1	3	27–	30	258	18	6	2	22–	14	77	20	4	1	104	96	345	22	3	0	75–	14	180	24	4	1	84	90	139	28	1	0	56–	38	0
17	2	0	253	254	90	18	7	0	216	213	180	20	4	2	53	47	229	22	3	1	92	64	37	24	4	2	100	91	277	28	1	1	28–	32	357
17	2	1	41–	32	292	18	7	1	30–	27	270	20	4	3	47	50	324	22	3	2	81	74	4	24	5	0	54–	40	0	28	2	0	51–	18	180
17	2	2	175	174	112	18	7	2	110	116	198	20	5	0	140	111	180	22	3	3	70	96	4	24	5	1	81	71	321	28	2	1	45	66	318
17	2	3	46	38	60	19	0	1	111	119	270	20	5	1	126	106	70	22	4	0	71–	4	180	24	6	0	36–	37	180	28	3	0	49	60	180
17	3	0	75–	17	90	19	0	2	31	41	0	20	5	2	50	34	211	22	4	1	106	89	74	24	6	1	15–	28	166	28	3	1	103	100	115
17	3	1	261	279	151	19	0	3	142	156	270	20	6	0	63–	65	180	22	4	2	45	36	125	25	0	1	75	69	90	28	4	0	31–	6	0
17	3	2	109	96	38	19	1	0	240	223	90	20	6	1	34–	46	289	22	5	0	147	105	0	25	0	2	74	70	0	29	0	1	24–	25	270
17	3	3	51	56	194	19	1	1	119	104	259	20	6	2	66	56	146	22	5	1	35–	41	146	25	1	0	71–	68	270	29	1	0	47–	49	270
17	4	0	77–	50	90	19	1	2	109	88	83	20	7	0	49–	16	0	22	5	2	62	58	11	25	1	1	38–	30	240	29	1	1	52	58	6
17	4	1	42–	53	94	19	1	3	53	52	274	20	7	1	46	50	157	22	6	0	53–	34	0	25	1	2	22–	19	176	29	2	0	42–	30	270
17	4	2	68	67	345	19	2	0	76–	109	270	21	0	1	43–	50	270	22	6	1	54	47	97	25	2	0	69–	82	90	29	2	1	56	61	330
17	4	3	102	110	72	19	2	1	124	120	34	21	0	2	35	52	0	22	7	0	33–	25	0	25	2	1	90	81	38	29	3	0	32–	56	90
17	5	0	77–	64	90	19	2	2	52	43	324	21	0	3	21–	25	270	23	0	1	42–	60	90	25	2	2	88	83	156	30	0	0	38–	7	0
17	5	1	52	73	336	19	2	3	37	29	135	21	1	0	105	130	90	23	0	2	142	145	180	25	3	0	65–	57	90	30	1	0	36–	2	0

The atomic scattering factors used throughout the calculations are those of Dawson (1960) for S and of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for Cl, O, N and C.

All the calculations were performed on the Olivetti Elea 6001/S computer of the *Centro di Calcolo Elettronico della Università di Parma* using the programs of Nardelli, Musatti, Domiano & Andreetti (1964, 1965) and the least-squares program of Sgarlata (1965).

Discussion

The X-ray analysis confirms the isothiazole structure already proposed from chemical evidence. A projection on (001) is shown in Fig. 1; the molecules are nearly planar and the dihedral angle they form with the projection plane is 25·6°. Bond distances and angles are quoted in Table 4.

There is a small but statistically significant departure from coplanarity for the two rings as indicated by the analysis of planarity for the molecule shown in Table 5. The dihedral angle between the benzene and isothiazole rings, as calculated from the least-squares equations, is 179·3°.

The oxygen atom lies in the isothiazole plane in agreement with the trigonal character of C(7). The chlorine atom is slightly out of the benzene plane (0·025 Å); this displacement, which is statistically significant, corresponds to a displacement, on the opposite side, of the sulphur atom (0·021 Å) from the same

Table 4. *Bond distances and angles with their e.s.d.'s*

Cl—C(1)	1·74 (1) Å	C(6)–C(1)	1·41 (1) Å
C(1)–C(2)	1·37 (1)	C(6)–S	1·72 (1)
C(2)–C(3)	1·42 (1)	S—N	1·68 (1)
C(3)–C(4)	1·38 (1)	N—C(7)	1·34 (1)
C(4)–C(5)	1·40 (1)	C(7)–O	1·22 (1)
C(5)–C(6)	1·39 (1)	C(7)–C(5)	1·48 (1)
Cl—C(1)–C(2)	120·9 (0·7)°	C(5)–C(6)–S	114·0 (0·6)°
Cl—C(1)–C(6)	118·1 (0·6)	C(6)–S—N	88·9 (0·3)
C(1)–C(2)–C(3)	119·3 (0·8)	S—N—C(7)	118·4 (0·6)
C(2)–C(3)–C(4)	121·2 (0·7)	N—C(7)–C(5)	108·5 (0·7)
C(3)–C(4)–C(5)	118·0 (0·8)	N—C(7)–O	123·9 (0·7)
C(4)–C(5)–C(6)	122·2 (0·7)	O—C(7)–C(5)	127·6 (0·7)
C(5)–C(6)–C(1)	118·3 (0·7)	C(7)–C(5)–C(4)	127·6 (0·7)
C(6)–C(1)–C(2)	121·0 (0·8)	C(7)–C(5)–C(6)	110·2 (0·6)
C(1)–C(6)–S	127·7 (0·7)		

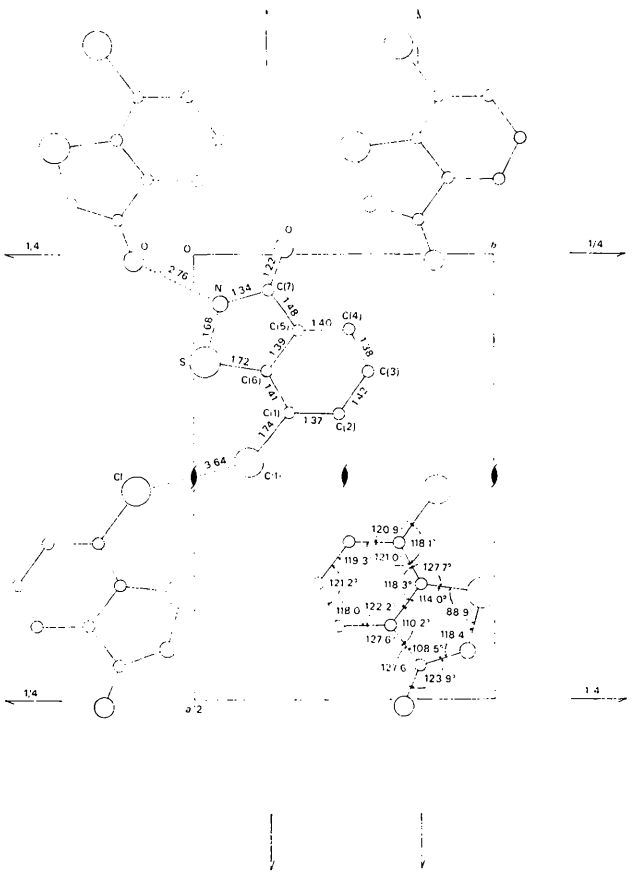

Fig.1. 7-Chloro-1,2-benzoisothiazolin-3-one; projection on (001).

plane. The Cl···S=3·282 (4) Å is appreciably shorter than the sum of the van der Waals radii (3·50 Å) calculated assuming a 1·70 Å value for the sulphur radius (the value usually given as 1·85 Å is too high as has been shown in many instances: Donohue, 1950; Ždanov & Zvonkova, 1950; van der Helm, Lessor & Merritt, 1960; Nardelli, Fava Gasparri, Giraldi Battistini & Domiano, 1966). This short intramolecular contact seems responsible for the small distortion of the molecule and probably is related to the lack of biological activity as found when the 7-position is occupied.

The C–C distances in the benzene ring are not significantly different from those usually found and the largest deviation of the angles from the 120° theoretical value is 2·2°. The C–Cl distance lies in the middle of the range of similar distances recently found in chlorine substituted benzenes: 1·76 in bis-(5-chlorosalicylaldoximato)copper(II) (Orioli, Lingafelter & Brown, 1964); 1·768 in *N*-methyl-*p*-chlorobenzaldoxime (Folting & Lipscomb, 1964); 1·73 in 1,6-di-*p*-chlorophenyl-3,4-dimethylhexatriene (Stam & Riva di Sanseverino, 1966) 1·717 in chloranilic acid (Andersen, 1967). The C(5)–C(7) distance corresponds to a single C(sp^2)–C(sp^2) bond and the C(7)–O distance agrees well with the generally given value for a C=O double bond. The other distances in the isothiazole ring all indicate some double bond character. The value of the C–S–N angle is in agreement with those generally found for sulphur in five-membered rings: 90·6° in phenylthiazolidinedione (Matthews, 1964); 90·6° in 1,4-bis(*N*-ethyl-1,2-dihydrobenzothiazol-2-ylidene)tetrazen (Allmann, 1967).

Packing, shown in the clinographic projection of Fig. 2 is essentially determined by the NH···O=2·76 (1) Å

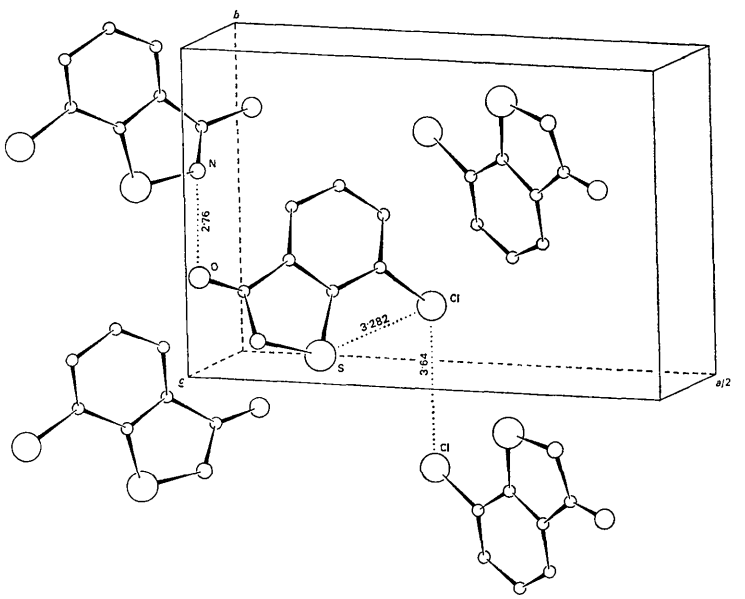

Fig.2. 7-Chloro-1,2-benzoisothiazolin-3-one; clinographic projection of a unit cell.

Table 5. *Analysis of the planarity of the molecule**

Best plane through	ClSONC(1)···C(7)		SONC(1)···C(7)		C(1)···C(6)		SONC(5)C(6)C(7)	
m_1	0·3849		0·3930		0·3921		0·3919	
m_2	0·2081		0·2084		0·2150		0·2037	
m_3	0·8992		0·8956		0·8944		0·8972	
d	2·6996		2·7119		2·7306		2·7083	
Atom $\sigma\perp$(Å)$\times 10^3$	Δ(Å)$\times 10^3$	$\Delta/\sigma\perp$	Δ(Å)$\times 10^3$	$\Delta/\sigma\perp$	Δ(Å)$\times 10^3$	$\Delta/\sigma\perp$	Δ(Å)$\times 10^3$	$\Delta/\sigma\perp$
Cl 3	7	2·3	(39)	(13·0)	(25)	(8·3)	(30)	(10·0)
S 2	−5	−2·5	0	0	(−22)	(−11·0)	1	0·5
O 7	27	3·9	6	0·9	(−1)	(−0·1)	2	0·3
N 8	−8	−1·0	−17	−2·1	(−35)	(−4·4)	−15	−1·9
C(1) 9	−2	−0·2	19	2·1	12	1·3	(6)	(0·7)
C(2) 10	−26	−2·6	−4	−0·4	−1	−0·1	(−23)	(−2·3)
C(3) 9	−23	−2·6	−11	−1·2	−2	−0·2	(−32)	(−3·6)
C(4) 8	−12	−1·5	−11	−1·4	−5	−0·6	(−27)	(−3·4)
C(5) 7	17	2·4	16	2·3	12	1·7	7	1·0
C(6) 7	−13	−1·9	−4	−0·6	−14	−2·0	−11	−1·6
C(7) 9	16	1·8	4	0·4	(−5)	(−0·6)	1	0·1
$\Sigma(\Delta/\sigma\perp)^2$		56·2		19·0		9·0		7·5
χ^2_{95}%		15·5		14·1		7·8		7·8

* Equation of the plane: $m_1x+m_2y+m_3z=d$; $\sigma\perp=\{m_1^2\sigma^2(x)+m_2^2\sigma^2(y)+m_3^2\sigma^2(z)\}^{1/2}$; the $\sigma\perp$ values do not change for the different planes. Data refering to atoms not considered in calculating the plane equation are given in parentheses.

hydrogen bonds and by the Cl···Cl=3·643 (7) Å van der Waals contacts. The Cl atoms are packed around a 2_1 axis.

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