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SHORT STRUCTURAL PAPERS

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2-(2,6-Dimethyl-phenyl)imino-3-(2-chloro-benzoyl) thiazolidine

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Abstract. $C_{18}H_{17}N_2OSCl$, orthorhombic, $P2_12_12_1$, $a=6{\cdot}518(3)$, $b=13{\cdot}547(6)$, $c=19{\cdot}314(8)$ Å; $V=1705{\cdot}4$ Å^3; $Z=4$; $D_x=1{\cdot}335$, $D_c=1{\cdot}323$ g cm^{-3}. The structure was solved by direct methods and Fourier techniques. An R of 0·095 was obtained for 1207 observed reflexions after least-squares refinement.

Introduction. The structure of the title compound (hereinafter ATOCL) was determined in order to find out whether the *o*-chlorobenzoyl group is bound to the endocyclic N(1) (Fig. 1) or to the exocyclic N(2) of the 2-iminothiazoline moiety. A preliminary communication (Argay, Kálmán, Tóth & Toldy, 1972) revealed that the *o*-chlorobenzoyl group is linked to the endocyclic N(1). This paper reports the complete structure analysis and gives the final atomic parameters.

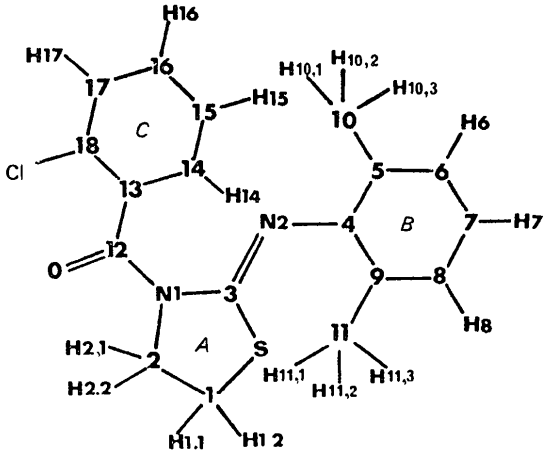

Fig. 1. Atomic numbering of the title compound. Unaccompanied numbers indicate carbon atoms. Rings are labelled *A*, *B* and *C*.

The crystals are colourless. Cell constants were determined from Weissenberg and precession photographs with Cu $K\bar{\alpha}$ ($\bar{\lambda}=1{\cdot}5418$ Å) radiation. The density was measured by flotation.

Intensities were collected on a Stoe semi-automatic two-circle diffractometer (for details see Kálmán, Simon, Schawartz & Horváth, 1974). Because of the small size of the crystal 970 (out of 1750) independent reflexions had $I-1{\cdot}5\sigma(I)<0$ and were taken as unobserved, with values of $I_o=\frac{1}{2}\sigma(I)$. The phase problem for 236 reflexions with $E>1{\cdot}50$ was solved with *MULTAN* (Main, Woolfson & Germain, 1971). The E map computed from the solution with the best ABSFOM = 1·11 revealed the positions of the Cl, S and a further six non-hydrogen atoms. Three cycles of structure-factor and Fourier calculations revealed the missing 15 non-hydrogen atoms ($R=0{\cdot}245$). Block-diagonal refinement of the atomic coordinates with isotropic and anisotropic thermal parameters resulted in a final R of 0·112 for the observed reflexions. The anisotropic refinement was then continued with new experimental data (1358 independent reflexions of which only 143 were unobserved) collected from a larger crystal on the same instrument.

The H atoms were located geometrically by comparison with a related compound, 2-(2,6-dimethylphenyl)imino-3-(2-methylbenzoyl)thiazolidine (hereinafter ATOME), the structure of which has recently been solved (Argay, Kálmán, Nahlovski & Ribár, 1975). The closing stage of the refinement, which was carried out for two separate groups of atoms (12 non-hydrogen

Table 1. *Final atomic positional* ($\times 10^4$ *for non-hydrogen atoms,* $\times 10^3$ *for hydrogen atoms*) *and vibrational parameters*

The estimated standard deviations (except for hydrogen atoms) are in parentheses. The b_{ij} are defined by

$$T=\exp\left[-10^4(b_{11}h^2+b_{22}k^2+b_{33}l^2+b_{12}hk+b_{13}hl+b_{23}kl)\right].$$

	x/a	y/b	z/c	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
S	3409 (5)	2443 (2)	2188 (1)	414 (7)	97 (2)	54 (1)	56 (7)	10 (5)	0 (1)
O	4974 (15)	1237 (7)	−85 (4)	437 (27)	118 (7)	52 (3)	−37 (25)	−7 (16)	−2 (7)
N(1)	4487 (14)	1606 (7)	1026 (5)	325 (23)	87 (6)	50 (3)	4 (23)	−26 (16)	8 (7)
N(2)	5234 (13)	646 (7)	2034 (4)	326 (19)	97 (5)	50 (2)	24 (20)	−5 (13)	6 (2)
C(1)	2489 (18)	3034 (8)	1390 (6)	436 (29)	91 (7)	65 (4)	100 (26)	−5 (21)	19 (9)
C(2)	3895 (22)	2639 (10)	820 (7)	422 (36)	94 (8)	55 (4)	49 (32)	2 (22)	14 (9)
C(3)	4478 (14)	1431 (8)	1760 (5)	271 (20)	100 (6)	50 (3)	−1 (24)	37 (14)	2 (3)
C(4)	5064 (15)	542 (7)	2752 (5)	329 (23)	74 (6)	51 (3)	37 (22)	11 (16)	12 (3)
C(5)	3487 (17)	−6 (8)	2983 (5)	370 (25)	97 (6)	51 (3)	58 (26)	8 (16)	18 (3)
C(6)	3297 (20)	−161 (10)	3725 (7)	453 (34)	125 (9)	66 (4)	76 (35)	15 (23)	11 (4)
C(7)	4769 (20)	230 (8)	4148 (5)	509 (34)	103 (7)	51 (3)	124 (29)	26 (21)	−1 (3)
C(8)	6363 (18)	733 (8)	3892 (6)	464 (31)	87 (7)	61 (3)	94 (27)	−13 (20)	2 (3)
C(9)	6522 (17)	933 (8)	3200 (5)	352 (26)	105 (7)	51 (3)	55 (27)	−4 (17)	−8 (3)
C(10)	1960 (20)	−507 (10)	2505 (6)	440 (32)	117 (8)	63 (4)	−72 (32)	−54 (20)	−2 (4)
C(11)	8271 (21)	1556 (10)	2914 (7)	443 (36)	124 (9)	71 (4)	−32 (38)	15 (23)	12 (4)
C(12)	5089 (16)	993 (8)	523 (5)	282 (24)	77 (6)	46 (3)	−39 (22)	7 (15)	−2 (7)
C(13)	5742 (18)	−43 (9)	678 (6)	301 (26)	91 (7)	50 (3)	−9 (27)	−3 (17)	12 (8)
C(14)	4459 (24)	−792 (10)	552 (7)	442 (40)	103 (9)	55 (4)	−15 (40)	−7 (23)	12 (10)
C(15)	5135 (26)	−1787 (11)	681 (8)	556 (47)	101 (10)	64 (5)	19 (44)	−22 (29)	12 (11)
C(16)	7094 (23)	−1964 (11)	896 (7)	487 (36)	104 (9)	57 (4)	31 (35)	−20 (24)	12 (11)
C(17)	8467 (23)	−1192 (10)	996 (7)	421 (37)	94 (9)	52 (4)	44 (35)	−1 (25)	−1 (10)
C(18)	7781 (19)	−244 (10)	881 (6)	295 (28)	98 (9)	55 (4)	7 (28)	12 (21)	3 (10)
Cl	9481 (5)	748 (3)	971 (2)	305 (7)	115 (2)	64 (1)	−58 (8)	2 (5)	−14 (3)

Table 1 (*cont.*)

	x/a	y/b	z/c	B_i
H(1,1)	123	269	150	5·2
H(1,2)	200	370	133	5·2
H(2,1)	517	305	81	5·7
H(2,2)	314	262	38	5·7
H(6)	215	−59	392	5·8
H(7)	461	20	468	5·6
H(8)	745	90	423	5·5
H(10,1)	100	−90	285	6·5
H(10,2)	120	−20	210	6·5
H(10,3)	280	−85	210	6·5
H(11,1)	785	220	268	6·5
H(11,2)	940	122	270	6·5
H(11,3)	910	210	300	6·5
H(14)	305	−64	38	4·6
H(15)	414	−235	63	5·7
H(16)	755	−265	99	6·5
H(17)	997	−130	115	5·8

atoms in each) with fixed H positions, yielded a final $R=0{\cdot}095$ for 1207 observed intensities (0·102 for all reflexions).*

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 30982 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Discussion. The atomic parameters are given in Table 1. The refinement based on the new data considerably improved the estimated standard deviations of the atomic parameters. The structure determination of ATOCL, however, is less accurate than that of ATOME. The bonding of the thiazolidine ring and of its environment is therefore presented with the discussion of the structure of ATOME (Argay, Kálmán, Nahlovski & Ribár, 1975).

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