

Table 1. Atomic fractional coordinates ($\times 10^4$) and U_{eq} ($\text{\AA}^2 \times 10^4$)

	x	y	z	U_{eq}^*
Cl	7415 (1)	-44 (1)	5570 (1)	725 (3)
O(1)	8474 (2)	4112 (2)	4075 (2)	641 (9)
O(2)	6657 (1)	3018 (2)	3974 (2)	481 (6)
C(1)	8146 (2)	1271 (2)	3698 (2)	388 (7)
C(2)	8015 (2)	-130 (2)	4353 (2)	432 (8)
C(3)	8408 (2)	-1634 (3)	4082 (3)	549 (10)
C(4)	8904 (2)	-1762 (3)	3136 (3)	571 (10)
C(5)	9037 (2)	-398 (3)	2469 (3)	557 (11)
C(6)	8680 (2)	1102 (3)	2770 (2)	473 (10)
C(7)	7803 (2)	2955 (2)	3954 (2)	410 (8)
C(8)	6185 (2)	4612 (3)	4186 (3)	459 (9)
C(9)	5239 (2)	4235 (3)	4777 (3)	543 (11)
C(10)	5664 (4)	5509 (4)	2888 (3)	718 (14)

* Hamilton (1959).

Table 2. Bond distances (\AA) and angles ($^\circ$)

Cl—C(2)	1.730 (3)	C(2)—C(3)	1.386 (3)
O(1)—C(7)	1.198 (3)	C(3)—C(4)	1.372 (5)
O(2)—C(7)	1.328 (3)	C(4)—C(5)	1.379 (4)
O(2)—C(8)	1.469 (3)	C(5)—C(6)	1.378 (4)
C(1)—C(2)	1.396 (3)	C(8)—C(9)	1.500 (5)
C(1)—C(6)	1.388 (4)	C(8)—C(10)	1.510 (4)
C(1)—C(7)	1.493 (3)	C(9)—C(9')	1.526 (4)
C(1)—C(7)	1.393 (3)		
C(7)—O(2)—C(8)	117.9 (1)	C(4)—C(5)—C(6)	119.4 (2)
C(6)—C(1)—C(7)	117.1 (2)	C(1)—C(6)—C(5)	121.6 (2)
C(2)—C(1)—C(7)	125.1 (2)	O(2)—C(7)—C(1)	112.1 (2)
C(2)—C(1)—C(6)	117.7 (2)	O(1)—C(7)—C(1)	123.2 (2)
Cl—C(2)—C(1)	121.5 (1)	O(1)—C(7)—O(2)	124.6 (2)
C(1)—C(2)—C(3)	120.8 (2)	O(2)—C(8)—C(10)	108.6 (2)
Cl—C(2)—C(3)	117.7 (1)	O(2)—C(8)—C(9)	105.1 (2)
C(2)—C(3)—C(4)	119.9 (2)	C(9)—C(8)—C(10)	115.0 (2)
C(3)—C(4)—C(5)	120.4 (2)	C(8)—C(9)—C(9')	112.5 (2)

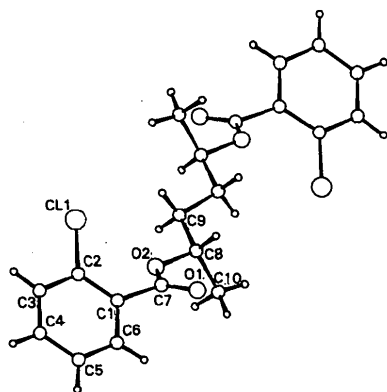


Fig. 1. Projection of the molecule.

Related literature. This compound is strictly related to the analogous derivatives with *para* and *meta* chlorines (Bocelli & Grenier-Loustalot, 1984) and to that without halogens (Bocelli & Grenier-Loustalot, 1982).

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Structure of Methyl (Z)-2-Cyano-3-[(*E*)- α -(methylthio)benzylideneamino]-3-phenylpropenoate

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Abstract. $C_{19}H_{16}N_2O_2S$, $M_r = 336.408$, monoclinic, $P2_1/n$, $a = 9.587$ (2), $b = 10.292$ (3), $c = 17.718$ (4) \AA , $\beta = 97.11$ (1) $^\circ$, $V = 1734.8$ (7) \AA^3 , $Z = 4$, $D_x =$

1.288 g cm^{-3} , Mo $K\alpha$, $\lambda = 0.7107$ \AA , $\mu = 1.897$ cm^{-1} , $F(000) = 704$, room temperature, final $R = 0.062$ and $wR = 0.055$ for 4028 observed reflections. In the

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central chain the values of the interatomic C—N [1.263 (2) Å] and C—C [1.367 (3) Å] distances and the C=N—C=C torsion angle [−80.9 (3)°], indicate a constrained electronic conjugation. The torsion angles about the two double bonds are 172.0 (2) and 7.6 (3)°, and the arrangements around these double bonds are (*E*) and (*Z*) respectively.

Experimental. Crystal 0.20 × 0.25 × 0.30 mm. Enraf–Nonius CAD-4 automatic diffractometer, 25 reflections used in determination of lattice parameters ($8 < \theta < 18^\circ$), no absorption correction. Data collection: Mo *K* α , $2 < \theta < 30^\circ$, *h* 0 to 13, *k* 0 to 14, *l* −24 to 24. Two check reflections ($2\bar{4}2$, $2\bar{4}\bar{2}$) measured every 100 reflections showed no significant variation; 5261 unique reflections, 4028 observed with $I > 2\sigma(I)$. $R_{\text{int}} = 0.019$. Structure solved by direct methods with *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980); refined by full-matrix least squares with $\sum w(|F_o| - |F_c|)^2$ minimized; unit weights since an applied weighting scheme (Martínez-Ripoll & Cano, 1975) gave no trends in F_o and $\sin \theta/\lambda$; anisotropic thermal parameters for non-H atoms.

All H atoms located in difference Fourier synthesis, positional parameters included in further refinement with fixed isotropic temperature factors equal to those of the atoms to which they are bonded. $\Delta\rho_{\text{max}} = 0.21$, $\Delta\rho_{\text{min}} = -0.23 \text{ e } \text{\AA}^{-3}$, $(\Delta/\sigma)_{\text{max}} = 0.015$. Final $R = 0.062$ and $wR = 0.055$, $S = 5.19$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Calculations performed with *XRAY70*

Table 2. Bond distances (Å), bond angles (°) and selected torsion angles (°) with *e.s.d.*'s in parentheses

S1—C2	1.738 (2)	C2—S1—C10	101.0 (1)
S1—C10	1.797 (3)	S1—C2—C21	113.6 (1)
C2—N3	1.263 (2)	S1—C2—N3	121.6 (2)
C2—C21	1.490 (3)	N3—C2—C21	124.9 (2)
N3—C4	1.373 (2)	C2—N3—C4	126.1 (2)
C4—C5	1.367 (3)	N3—C4—C41	114.4 (2)
C4—C41	1.479 (3)	N3—C4—C5	121.7 (2)
C5—C6	1.493 (3)	C5—C4—C41	123.7 (2)
C5—C51	1.433 (3)	C4—C5—C51	121.0 (2)
C6—O7	1.333 (3)	C5—C6—O7	110.5 (2)
C6—O9	1.195 (3)	C5—C6—O9	126.3 (2)
C8—O7	1.451 (3)	C5—C51—N52	177.9 (2)
C21—C22	1.390 (3)	C6—O7—C8	116.2 (2)
C21—C26	1.389 (3)	O7—C6—O9	123.2 (2)
C22—C23	1.387 (4)		
C23—C24	1.386 (4)	C10—S1—C2—N3	−7.8 (2)
C24—C25	1.377 (4)	S1—C2—N3—C4	172.0 (2)
C25—C26	1.402 (4)	C21—C2—N3—C4	−8.9 (3)
C41—C42	1.397 (3)	C2—N3—C4—C5	−80.9 (3)
C41—C46	1.397 (3)	C2—N3—C4—C41	104.7 (2)
C42—C43	1.395 (4)	C4—C5—C6—O7	−173.4 (2)
C43—C44	1.381 (4)	C4—C5—C6—O9	6.6 (4)
C44—C45	1.386 (5)	N3—C4—C5—C51	−166.8 (2)
C45—C46	1.393 (4)	C41—C4—C5—C51	7.1 (3)
C51—N52	1.137 (3)		

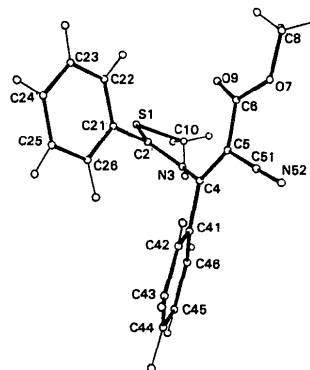


Fig. 1. A view of the molecule with the atomic labelling.

Table 1. Fractional coordinates and equivalent isotropic thermal parameters (Å²)

$$U_{\text{eq}} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j \cos(\mathbf{a}_i, \mathbf{a}_j).$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
S1	0.1251 (1)	0.7267 (1)	0.4004 (1)	0.0483 (2)
C2	0.1824 (2)	0.6764 (2)	0.4927 (1)	0.0370 (5)
N3	0.2919 (2)	0.6084 (2)	0.5079 (1)	0.0430 (5)
C4	0.3549 (2)	0.5764 (2)	0.5793 (1)	0.0392 (5)
C5	0.4420 (2)	0.6609 (2)	0.6219 (1)	0.0410 (5)
C6	0.4625 (2)	0.7986 (2)	0.5992 (1)	0.0466 (6)
O7	0.5637 (2)	0.8545 (2)	0.6466 (1)	0.0642 (6)
C8	0.5957 (3)	0.9887 (3)	0.6304 (2)	0.0759 (11)
O9	0.3992 (2)	0.8539 (2)	0.5464 (1)	0.0752 (7)
C10	0.2701 (3)	0.6765 (3)	0.3520 (2)	0.0695 (10)
C21	0.0896 (2)	0.7197 (2)	0.5494 (1)	0.0385 (5)
C22	0.0645 (2)	0.8512 (2)	0.5595 (1)	0.0501 (7)
C23	−0.0201 (3)	0.8908 (3)	0.6133 (1)	0.0636 (9)
C24	−0.0817 (3)	0.7984 (3)	0.6555 (1)	0.0673 (9)
C25	−0.0583 (3)	0.6680 (3)	0.6452 (2)	0.0651 (9)
C26	0.0289 (2)	0.6267 (2)	0.5919 (1)	0.0508 (9)
C41	0.3312 (2)	0.4407 (2)	0.6020 (1)	0.0425 (6)
C42	0.3119 (3)	0.4098 (3)	0.6768 (1)	0.0572 (8)
C43	0.2787 (3)	0.2828 (3)	0.6955 (2)	0.0724 (10)
C44	0.2662 (3)	0.1867 (3)	0.6407 (2)	0.0764 (11)
C45	0.2852 (3)	0.2165 (3)	0.5664 (2)	0.0730 (10)
C46	0.3168 (3)	0.3432 (2)	0.5467 (1)	0.0560 (7)
C51	0.5295 (2)	0.6179 (2)	0.6887 (1)	0.0442 (6)
N52	0.6023 (2)	0.5860 (2)	0.7410 (1)	0.0594 (7)

(Stewart, Kundell & Baldwin, 1970), *PARST* (Nardelli, 1983) and *PESOS* (Martínez-Ripoll & Cano, 1975) on a UNIVAC 1108 computer.

The structure of the title compound together with the atomic labelling scheme is shown in Fig. 1. Positional parameters and the equivalent *U* values of the anisotropic temperature factors are given in Table 1.* Bond lengths and angles and selected torsion angles are given in Table 2.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43779 (39 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Related literature. 2-[α -(Methylthio)benzylidene-amino]-2-phenyl-1,1-ethylenedicarbonitrile (Balcazar, Florencio & García-Blanco, 1985; Yeh, Moriarty, Yeh & Ramey, 1972).

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Benzyl-9 Diméthyl-1,4 Diméthylamino-6 Carbazoledicarbaldéhyde-3,5

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Abstract. $C_{25}H_{24}N_2O_2$, $M_r = 384.5$, triclinic, $P\bar{1}$, $a = 9.860$ (3), $b = 10.953$ (2), $c = 12.304$ (2) Å, $\alpha = 125.60$ (2), $\beta = 95.25$ (2), $\gamma = 105.54$ (2)°, $V = 987.5$ Å³, $Z = 2$, $D_m = 1.27$, $D_x = 1.293$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.7107$ Å, $\mu = 0.077$ mm⁻¹, $F(000) = 408$, room temperature, $R = 0.051$ for 1536 independent reflections [$I > 3\sigma(I)$]. The structure was solved as it was impossible to infer the positions occupied by the two formyl groups from the NMR spectroscopy. The steric hindrance entails a distortion of the carbazole group which is not as planar as it is in the carbazole molecule. The distances from the atoms of the carbazole group to its mean plane are ≤ 0.216 (4) Å. The phenyl ring of the benzyl group and the pyrrole ring are almost perpendicular [85.7 (2)°]. The molecules form columns parallel to the [010] axis.

Partie expérimentale. Masse volumique par flottaison. Cristal prismatique: 0,12 × 0,20 × 0,30 mm. Dimensions de la maille déterminées sur monocristal avec 25 réflexions telles que $6,23 \leq \theta \leq 13,64^\circ$. Diffractomètre Enraf-Nonius CAD-4. $0 \leq (\sin \theta) / \lambda \leq 0,550$ Å⁻¹; -10

$\leq h \leq 10$, $0 \leq k \leq 11$, $-13 \leq l \leq 10$. Réflexions de contrôle: $\bar{3}\bar{3}5$, 120 et $23\bar{3}$. $\sigma(I)/I$ (contrôle) = 6×10^{-3} . Diminution de I : 1,0%. 2751 réflexions indépendantes mesurées, 1215 réflexions inobservées [$I \leq 3\sigma(I)$].

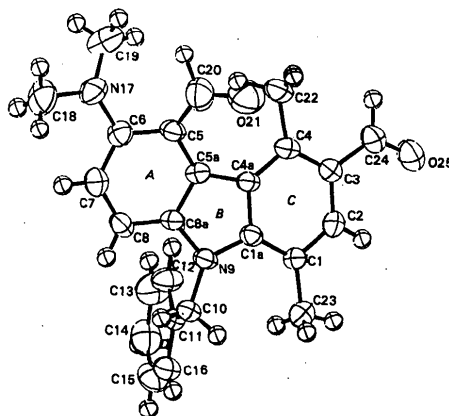


Fig. 1. Vue de la molécule en perspective, numérotation des atomes et lettres utilisées pour désigner les cycles.