

atomic coordinates,* Table 2 displays the bond lengths and angles, and Fig. 1 shows a view of the molecule with the numbering used in the crystallographic study.

Related literature. Structure of 2-[*o*-(methylthio)benzylideneamino]-2-phenyl-1,1-ethylenedicarbonitrile (Balcazar, Florencio & García-Blanco, 1985) and tandem [2,3]sigmatropic rearrangement of a sulfonium ylide and cyclopropanation of the resulting electron-rich olefin on a 4-methoxy-2-pyrone derivative (de March, Moreno-Manas, Ripoll, Florencio, García-Blanco & Martínez-Carrera, 1986).

* 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 43778 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of 2-Methylthio-2-[α -(methylthio)ethylideneamino]-1,1-ethylenedicarbonitrile

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Abstract. $C_8H_9N_3S_2$, $M_r = 211.30$, triclinic, $P\bar{1}$, $a = 10.489$ (4), $b = 14.230$ (9), $c = 7.790$ (4) Å, $\alpha = 94.74$ (1), $\beta = 110.36$ (1), $\gamma = 86.34$ (1)°, $V = 1085.6$ (9) Å³, $Z = 4$, $D_x = 1.293$ g cm⁻³, Mo $K\alpha$, $\lambda = 0.7107$ Å, $\mu = 4.315$ cm⁻¹, $F(000) = 440$, room temperature, final $R = 0.054$ and $wR = 0.069$ for 5174 observed reflections. The configuration at the C=N bond is (*E*). The C–C(CN)₂ groups are nearly planar. The torsion angles C=N–C=C are 80.6 (3) and –84.1 (3)° respectively on the two independent molecules.

Experimental. Crystal 0.40 × 0.35 × 0.50 mm. Enraf–Nonius CAD-4 automatic diffractometer, 25 reflections used in determination of lattice parameters ($8 < \theta < 13^\circ$), absorption correction (transmission factors 0.62–1.36). Data collection: Mo $K\alpha$, $2 < \theta < 30^\circ$, $h = -14$ to 14, $k = 0$ to 14, $l = -10$ to 10. Two check reflections ($\bar{2}15$, $10\bar{7}$) measured every 100 reflections showed no significant variation; 6166 unique reflections measured, 5174 observed with $I > 2\sigma(I)$. $R_{int} = 0.085$. Structure solved by direct methods with *MULTAN80* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson,

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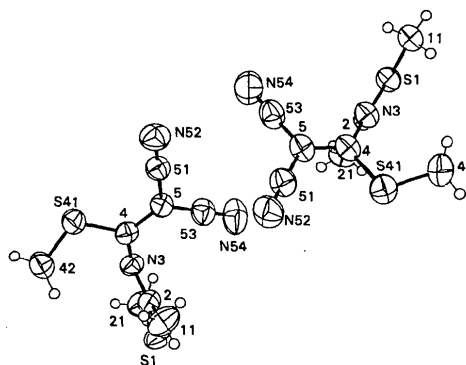


Table 1. Fractional coordinates and equivalent isotropic thermal parameters ($\text{\AA}^2 \times 10^4$)
$$U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j \cos(\mathbf{a}_i, \mathbf{a}_j).$$

Molecule (1)	x	y	z	U_{eq}
S1	0.5593 (1)	-0.1219 (1)	0.3551 (1)	687 (3)
C11	0.6059 (3)	-0.0914 (3)	0.1677 (4)	768 (11)
C2	0.7048 (2)	-0.0957 (1)	0.5444 (3)	536 (7)
C21	0.6976 (4)	-0.1214 (3)	0.7224 (4)	824 (13)
N3	0.8045 (2)	-0.0570 (1)	0.5235 (2)	512 (5)
C4	0.9264 (2)	-0.0411 (1)	0.6622 (2)	484 (6)
S41	0.9651 (1)	0.0728 (1)	0.7570 (1)	592 (2)
C42	0.8091 (3)	0.1377 (2)	0.6454 (4)	694 (10)
C5	1.0242 (2)	-0.1126 (1)	0.7138 (3)	514 (6)
C51	1.1545 (2)	-0.0983 (1)	0.8511 (3)	539 (7)
N52	1.2586 (2)	-0.0872 (2)	0.9629 (3)	715 (8)
C53	0.9975 (2)	-0.2039 (2)	0.6224 (3)	627 (8)
N54	0.9775 (3)	-0.2767 (2)	0.5472 (4)	913 (11)

Molecule (2)	x	y	z	U_{eq}
S1	1.4055 (1)	-0.6096 (1)	0.4709 (1)	556 (2)
C11	1.5551 (3)	-0.6334 (2)	0.6652 (4)	657 (9)
C2	1.3001 (2)	-0.5487 (1)	0.5735 (2)	466 (6)
C21	1.1659 (2)	-0.5161 (2)	0.4393 (3)	606 (8)
N3	1.3375 (2)	-0.5358 (1)	0.7478 (2)	533 (6)
C4	1.2548 (2)	-0.4900 (1)	0.8337 (2)	523 (6)
S41	1.1639 (1)	-0.5556 (1)	0.9263 (1)	683 (3)
C42	1.2262 (4)	-0.6740 (2)	0.8995 (5)	770 (12)
C5	1.2473 (2)	-0.3933 (2)	0.8576 (3)	570 (7)
C51	1.1639 (3)	-0.3490 (2)	0.9530 (3)	624 (8)
N52	1.0942 (3)	-0.3150 (2)	1.0273 (4)	833 (11)
C53	1.3224 (3)	-0.3347 (2)	0.7910 (4)	678 (9)
N54	1.3825 (3)	-0.2881 (2)	0.7385 (4)	965 (4)

Table 2. Bond lengths (\AA), bond angles ($^\circ$) and selected torsion angles ($^\circ$)

	Molecule (1)	Molecule (2)	Average
S1—C2	1.749 (2)	1.729 (2)	1.739 (2)
S1—C11	1.785 (4)	1.798 (2)	1.792 (3)
C2—C21	1.491 (5)	1.504 (3)	1.498 (4)
C2—N3	1.277 (3)	1.276 (3)	1.277 (3)
N3—C4	1.374 (2)	1.373 (3)	1.374 (3)
C4—S41	1.735 (2)	1.734 (3)	1.735 (3)
C4—C5	1.377 (3)	1.374 (3)	1.376 (3)
S41—C42	1.799 (3)	1.790 (3)	1.795 (3)
C5—C51	1.427 (3)	1.421 (4)	1.424 (4)
C5—C53	1.424 (3)	1.424 (4)	1.424 (4)
C51—N52	1.146 (3)	1.143 (4)	1.145 (4)
C53—N54	1.141 (3)	1.132 (5)	1.137 (4)

C11—S1—C2	102.5 (2)	102.0 (1)	102.3 (2)
S1—C2—N3	120.3 (2)	120.6 (2)	120.5 (2)
S1—C2—C21	114.0 (2)	113.7 (2)	113.9 (2)
C21—C2—N3	125.7 (3)	125.7 (2)	125.7 (3)
C2—N3—C4	124.0 (2)	122.1 (2)	123.1 (2)
N3—C4—C5	120.7 (2)	122.0 (2)	121.4 (2)
N3—C4—S41	119.7 (2)	119.3 (2)	119.5 (2)
S41—C4—C5	119.2 (2)	118.6 (2)	118.9 (2)
C4—S41—C42	102.0 (2)	103.3 (2)	102.8 (2)
C4—C5—C53	119.3 (2)	121.9 (3)	120.3 (3)
C4—C5—C51	122.7 (3)	120.1 (3)	121.8 (3)
C51—C5—C53	118.0 (2)	118.0 (3)	118.0 (3)
C5—C51—N52	179.2 (3)	178.2 (3)	178.7 (3)
C5—C53—N54	178.7 (3)	179.8 (3)	179.3 (3)

S1—C2—N3—C4	-174.6 (2)	-178.2 (2)
C21—C2—N3—C4	6.2 (5)	0.9 (4)
C2—N3—C4—S41	-106.2 (3)	99.5 (3)
C2—N3—C4—C5	80.6 (3)	-84.1 (3)
N3—C4—C5—C51	177.1 (2)	-177.8 (3)
N3—C4—C5—C53	-0.4 (4)	1.5 (4)
N3—C4—S41—C42	5.9 (3)	6.5 (3)
S41—C4—C5—C51	3.9 (4)	-1.4 (4)
S41—C4—C5—C53	-173.6 (2)	177.9 (2)
C5—C4—S41—C42	179.2 (2)	-170.0 (2)

with fixed isotropic temperature factors, $(\Delta/\sigma)_{\max} = 0.040$. ρ_{\max} and $\rho_{\min} -0.31 \text{ e \AA}^{-3}$. Final $R = 0.054$ and $wR = 0.069$. Atomic scattering factors from

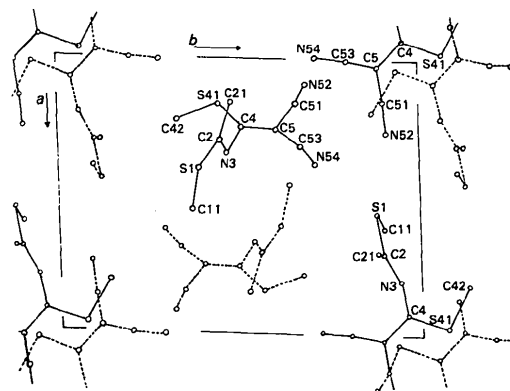


Fig. 2. Projection of the structure on the (001) plane.

International Tables for X-ray Crystallography (1974). Calculations performed with *XRAY70* (Stewart, Kundell & Baldwin, 1970), *PARST* (Nardelli, 1983) and *PESOS* (Martinez-Ripoll & Cano, 1975).

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. Fig. 2 shows a projection of the structure.

Related literature. Bond distances are comparable with those found in 2-[α -(methylthio)benzylideneamino]-2-phenyl-1,1-ethylenedicarbonitrile (Balcazar, Florencio & García-Blanco, 1985) and in (3*E*,5*Z*,7*Z*)-8-(diphenylmethylene)amino-3,5,7-octatrien-2-one (Wong, 1978).

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