C4	0.1961 (10)	0.9789 (5)	0.3036 (5)	0.079 (6)
C45	0.2581 (8)	0.7488 (6)	0.2609 (5)	0.077 (6)
C8	0.1655 (9)	0.7286 (7)	0.2198 (5)	0.076 (6)
C7	0.0907 (9)	0.7910 (7)	0.2045 (5)	0.085 (7)
C6	0.0992 (10)	0.8741 (8)	0.2298 (5)	0.090 (7)
C5	0.1886 (9)	0.8922 (6)	0.2717 (4)	0.069 (5)
O9	0.1461 (6)	0.6531 (5)	0.1929 (3)	0.089 (4)
C10	0.2167 (10)	0.5836 (7)	0.2099 (4)	0.087 (7)
C11	0.2020 (9)	0.5493 (6)	0.2785 (4)	0.074 (6)
C44	0.2909 (9)	0.5083 (7)	0.3082 (6)	0.083 (6)
C43	0.2768 (8)	0.4737 (6)	0.3666 (5)	0.079 (6)
C14	0.1761 (7)	0.4806 (5)	0.4008 (4)	0.061 (4)
C13	0.0899 (8)	0.5249 (6)	0.3707 (5)	0.075 (5)
C12	0.1047 (8)	0.5559 (6)	0.3121 (5)	0.075 (6)
C15	0.1630 (7)	0.4472 (5)	0.4667 (4)	0.057 (4)
C16	0.2099 (7)	0.3710 (6)	0.4867 (5)	0.072 (5)
C42	0.1092 (8)	0.4954 (5)	0.5127 (4)	0.060 (4)
C20	0.0396 (7)	0.5248 (5)	0.6225	0.056 (4)
S31	0.0652 (2)	1.0987 (1)	0.5611 (1)	0.077 (1)
O25	−0.0487 (6)	0.7740 (3)	0.7612 (3)	0.069 (3)
C41	−0.0551 (7)	0.5736 (5)	0.6063 (4)	0.062 (5)
C40	−0.1056 (8)	0.6289 (6)	0.6494 (4)	0.069 (5)
C26	−0.0520 (8)	0.8272 (5)	0.7095 (4)	0.059 (4)
C21	0.0835 (8)	0.5342 (5)	0.6855 (4)	0.067 (5)
C33	0.2547 (8)	1.1066 (5)	0.4818 (4)	0.068 (5)
C17	0.1990 (9)	0.3436 (6)	0.5504 (6)	0.088 (6)
C23	−0.0642 (7)	0.6367 (5)	0.7099 (4)	0.063 (5)
C19	0.0976 (7)	0.4700 (4)	0.5756 (4)	0.059 (4)
C38	−0.1372 (8)	0.9110 (7)	0.6256 (5)	0.081 (6)
C24	−0.1149 (8)	0.6987 (5)	0.7569 (4)	0.072 (5)
C22	0.0321 (8)	0.5902 (5)	0.7279 (4)	0.065 (5)
C39	−0.1461 (8)	0.8454 (7)	0.6738 (5)	0.078 (6)
C32	0.1863 (9)	1.0477 (6)	0.5254 (4)	0.083 (6)
C29	−0.0395 (8)	0.9495 (6)	0.6116 (5)	0.072 (5)
C34	0.3557 (10)	1.1443 (8)	0.5013 (6)	0.091 (7)
C30	−0.0380 (9)	1.0141 (7)	0.5591 (7)	0.098 (8)
C35	0.4183 (10)	1.1948 (8)	0.4603 (8)	0.109 (9)
C18	0.1451 (9)	0.3939 (6)	0.5940 (4)	0.074 (5)
C27	0.0474 (8)	0.8699 (7)	0.6957 (5)	0.078 (6)
C28	0.0528 (9)	0.9316 (7)	0.6498 (5)	0.086 (7)
O47	0.3337 (10)	0.8410 (7)	0.4587 (5)	0.148 (4)
O48	0.3079 (11)	0.6683 (8)	0.4418 (7)	0.168 (4)
O49	0.1701 (16)	0.7709 (12)	0.5312 (11)	0.255 (8)

Table 2. *Selected geometric parameters (Å)*

S3—C2	1.78 (1)	S31—C32	1.79 (1)
S3—C4	1.81 (1)	S31—C30	1.80 (1)
C8—O9	1.34 (1)	O25—C26	1.37 (1)
O9—C10	1.42 (1)	O25—C24	1.42 (1)

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *SDP* (Enraf–Nonius, 1985). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELX*76 (Sheldrick, 1976). Molecular graphics: *PLUTO* (Motherwell & Clegg, 1978); *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *PARST* (Nardelli, 1983).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: PT1030). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Ethyl Cyano(4-oxo-3-phenyl-1,3-thiazolidin-2-ylidene)acetate

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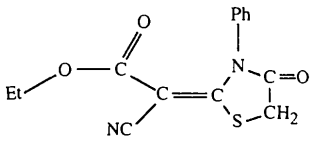
Abstract

There are two crystallographically independent but chemically equivalent molecules present in the asymmetric unit of the title compound, $C_{14}H_{12}N_2O_3S$. There are no unusual intra- or intermolecular distances or angles. The crystal packing is dominated mainly by hydrogen bonds and all rings in the molecules are essentially planar.

Comment

The X-ray structure analysis of the title compound, (I), was undertaken in order to confirm the structure proposed from spectroscopy studies (González, Enriquez, Castañedo & Kellin, 1990). This compound shows strong possible activity as an adrenergic β-blocker, hypotensor and cardiotonic agent based on the results

obtained from the *OREX* system (Institute for Organic Synthesis, 1990) for predicting the possible bioactive properties of small molecules.



(I)

There are two formula units of the title compound in the asymmetric unit. The molecules are packed along the [001] direction to form an extensive network *via* two weak hydrogen bonds (Nyburg & Faerman, 1985; Sutor, 1962): H(16*A*)···O(1*A*^{i}) 2.509 (8) Å, C(16*A*)—H(16*A*)···O(1*A*^{i}) 141.30 (19)°; H(10*B*)···O(2*A*) 2.593 (1) Å, C(10*B*)—H(10*B*)···O(2^{ii}) 152.23 (15)° [symmetry codes: (i) x, $\frac{1}{2}-y$, $\frac{1}{2}+z$; (ii) $-x$, $\frac{1}{2}+y$, $\frac{1}{2}-z$]. All rings in the molecules are essentially planar. The thiazole ring has a mean out-of-plane deviation of 0.0381 Å in molecule *A* (0.0137 Å in molecule *B*), while the six-atom ring plane has a mean out-of-plane deviation of 0.0025 Å in molecule *A* (0.0017 Å in molecule *B*). The atom-numbering scheme is shown in Fig. 1.

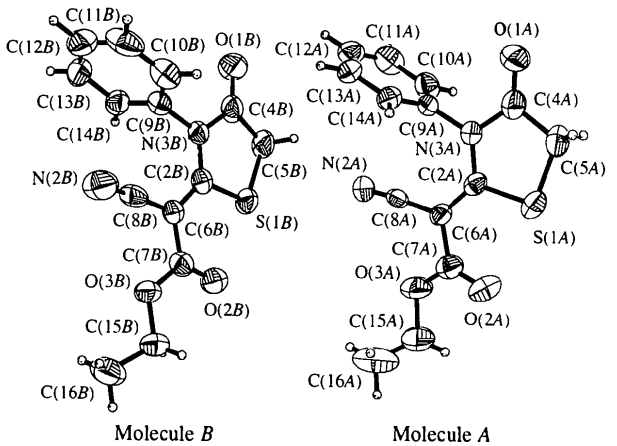


Fig. 1. View (*SHELXTL-Plus*; Sheldrick, 1991) of the two independent molecules in the asymmetric unit. Displacement ellipsoids are plotted at the 50% probability level.

Experimental

The title compound was obtained as described elsewhere (González, Dandaroba, Castañedo, Bermello & Rocha, 1996) from the reaction of 2,4-bis(carboethoxycyanomethylene)-1,3-dithietane (suspended in chloroform) with amine and phenyl isocyanate. The salt of the amine was filtered and washed with chloroform (González *et al.*, 1996). Bright yellow crystals were grown by slow evaporation from ethanol.

Crystal data

$C_{14}H_{12}N_2O_3S$
M_r = 288.32
Monoclinic
$P2_1/c$
a = 9.811 (3) Å
b = 12.845 (2) Å
c = 22.107 (3) Å
β = 96.65 (3)°
V = 2767.2 (10) Å^3
Z = 8
D_x = 1.384 Mg m^{-3}
D_m = 1.370 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 41 reflections
θ = 7.8–10.2°
μ = 0.23 mm^{-1}
T = 293 (2) K
Laminar
0.55 × 0.18 × 0.13 mm
Light yellow

Data collection

Siemens *P3/PC* diffractometer
$\theta/2\theta$ scans
Absorption correction: ψ scan (North, Phillips & Mathews, 1968)
T_{min} = 0.90, T_{max} = 1.00
5183 measured reflections
4875 independent reflections
2176 observed reflections [$I > 2\sigma(I)$]
R_{int} = 0.0332
θ_{max} = 25.0°
h = 0 → 11
k = 0 → 15
l = −26 → 26
3 standard reflections monitored every 100 reflections
intensity decay: <2%

Refinement

Refinement on F^2
$R(F)$ = 0.060
$wR(F^2)$ = 0.114
S = 1.12
4873 reflections
362 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 1.7550P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.048
$\Delta\rho_{max}$ = 0.224 e Å^{-3}
$\Delta\rho_{min}$ = −0.246 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
S(1A)	0.0728 (1)	0.0529 (1)	0.2692 (1)	0.055 (1)
O(1A)	0.0083 (5)	0.0799 (3)	0.0953 (2)	0.094 (2)
O(2A)	−0.0083 (4)	0.1311 (3)	0.3718 (2)	0.073 (1)
O(3A)	−0.1898 (5)	0.2359 (4)	0.3754 (2)	0.097 (2)
N(2A)	−0.3212 (5)	0.3281 (3)	0.2471 (2)	0.060 (1)
N(3A)	−0.0675 (4)	0.1502 (3)	0.1802 (2)	0.043 (1)
C(2A)	−0.0531 (5)	0.1437 (3)	0.2428 (2)	0.040 (1)
C(4A)	0.0096 (6)	0.0808 (4)	0.1492 (3)	0.060 (2)
C(5A)	0.0910 (5)	0.0100 (4)	0.1936 (2)	0.060 (2)
C(6A)	−0.1276 (5)	0.1989 (3)	0.2807 (2)	0.042 (1)
C(7A)	−0.0997 (6)	0.1846 (4)	0.3466 (2)	0.054 (1)
C(8A)	−0.2356 (6)	0.2702 (4)	0.2601 (2)	0.044 (1)
C(9A)	−0.1564 (5)	0.2233 (4)	0.1447 (2)	0.041 (1)
C(10A)	−0.2829 (5)	0.1904 (4)	0.1200 (2)	0.054 (1)
C(11A)	−0.3659 (6)	0.2590 (5)	0.0845 (2)	0.067 (2)
C(12A)	−0.3228 (6)	0.3578 (5)	0.0748 (2)	0.065 (2)
C(13A)	−0.1952 (6)	0.3898 (4)	0.1007 (2)	0.060 (2)
C(14A)	−0.1107 (5)	0.3224 (4)	0.1355 (2)	0.047 (1)
C(15A)	−0.1684 (9)	0.2375 (6)	0.4412 (3)	0.114 (3)
C(16A)	−0.1500 (8)	0.3392 (6)	0.4631 (3)	0.121 (3)

S(1*B*)	−0.4697 (2)	0.5732 (1)	0.2594 (1)	0.061 (1)
O(1*B*)	−0.5195 (4)	0.5936 (3)	0.0844 (2)	0.084 (1)
O(2*B*)	−0.3511 (4)	0.6680 (3)	0.3578 (2)	0.074 (1)
O(3*B*)	−0.2503 (3)	0.8250 (3)	0.3615 (1)	0.054 (1)
N(2*B*)	−0.2136 (5)	0.9206 (4)	0.2270 (2)	0.085 (2)
N(3*B*)	−0.4266 (4)	0.6876 (3)	0.1675 (2)	0.044 (1)
C(2*B*)	−0.4009 (5)	0.6849 (3)	0.2296 (2)	0.042 (1)
C(4*B*)	−0.4942 (6)	0.6006 (4)	0.1384 (3)	0.058 (2)
C(5*B*)	−0.5276 (6)	0.5236 (4)	0.1847 (2)	0.066 (2)
C(6*B*)	−0.3296 (5)	0.7583 (4)	0.2660 (2)	0.042 (1)
C(7*B*)	−0.3130 (5)	0.7435 (4)	0.3322 (2)	0.051 (1)
C(8*B*)	−0.2668 (5)	0.8483 (4)	0.2426 (2)	0.052 (1)
C(9*B*)	−0.3985 (5)	0.7750 (4)	0.1298 (2)	0.043 (1)
C(10*B*)	−0.2893 (6)	0.7730 (5)	0.0969 (3)	0.067 (2)
C(11*B*)	−0.2682 (7)	0.8579 (6)	0.0595 (3)	0.086 (2)
C(12*B*)	−0.3571 (8)	0.9403 (5)	0.0562 (3)	0.083 (2)
C(13*B*)	−0.4649 (7)	0.9405 (4)	0.0887 (3)	0.068 (2)
C(14*B*)	−0.4878 (5)	0.8583 (4)	0.1261 (2)	0.052 (1)
C(15*B*)	−0.2234 (6)	0.8154 (4)	0.4277 (2)	0.070 (2)
C(16*B*)	−0.1820 (7)	0.9185 (5)	0.4530 (3)	0.088 (2)

Table 2. *Selected geometric parameters (Å, °)*

S(1*A*)—C(2*A*)	1.749 (5)	O(2*B*)—C(7*B*)	1.203 (6)
S(1*A*)—C(5*A*)	1.788 (5)	O(3*B*)—C(7*B*)	1.343 (5)
O(1*A*)—C(4*A*)	1.191 (6)	O(3*B*)—C(15*B*)	1.461 (6)
O(2*A*)—C(7*A*)	1.212 (6)	N(2*B*)—C(8*B*)	1.139 (6)
O(3*A*)—C(7*A*)	1.324 (6)	N(3*B*)—C(2*B*)	1.366 (6)
O(3*A*)—C(15*A*)	1.445 (6)	N(3*B*)—C(4*B*)	1.416 (6)
N(2*A*)—C(8*A*)	1.133 (6)	N(3*B*)—C(9*B*)	1.443 (6)
N(3*A*)—C(2*A*)	1.376 (5)	C(2*B*)—C(6*B*)	1.376 (6)
N(3*A*)—C(4*A*)	1.400 (6)	C(4*B*)—C(5*B*)	1.487 (7)
N(3*A*)—C(9*A*)	1.449 (5)	C(6*B*)—C(8*B*)	1.434 (7)
C(2*A*)—C(6*A*)	1.371 (6)	C(9*B*)—C(14*B*)	1.380 (6)
C(4*A*)—C(5*A*)	1.499 (7)	C(10*B*)—C(11*B*)	1.397 (8)
C(6*B*)—C(7*B*)	1.467 (6)	C(11*B*)—C(12*B*)	1.368 (9)
C(9*B*)—C(10*B*)	1.363 (7)	C(15*B*)—C(16*B*)	1.476 (7)
C(6*A*)—C(8*A*)	1.435 (7)	C(15*A*)—C(16*A*)	1.398 (9)
C(6*A*)—C(7*A*)	1.463 (7)	S(1*B*)—C(2*B*)	1.748 (5)
C(9*A*)—C(10*A*)	1.364 (6)	S(1*B*)—C(5*B*)	1.800 (5)
C(9*A*)—C(14*A*)	1.373 (6)	O(1*B*)—C(4*B*)	1.195 (6)
C(10*A*)—C(11*A*)	1.381 (7)	C(13*B*)—C(14*B*)	1.375 (7)
C(12*B*)—C(13*B*)	1.346 (8)	C(12*A*)—C(13*A*)	1.378 (7)
C(11*A*)—C(12*A*)	1.362 (8)	C(13*A*)—C(14*A*)	1.372 (6)
C(2*A*)—S(1*A*)—C(5*A*)	92.1 (2)	O(2*A*)—C(7*A*)—O(3*A*)	124.2 (5)
C(7*A*)—O(3*A*)—C(15*A*)	117.6 (5)	O(2*A*)—C(7*A*)—C(6*A*)	124.8 (5)
C(2*A*)—N(3*A*)—C(4*A*)	117.1 (4)	O(3*A*)—C(7*A*)—C(6*A*)	111.0 (5)
C(2*A*)—N(3*A*)—C(9*A*)	124.7 (4)	N(2*A*)—C(8*A*)—C(6*A*)	176.0 (5)
C(4*A*)—N(3*A*)—C(9*A*)	118.2 (4)	C(10*A*)—C(9*A*)—C(14*A*)	121.8 (5)
C(6*A*)—C(2*A*)—N(3*A*)	125.7 (4)	C(10*A*)—C(9*A*)—N(3*A*)	118.6 (4)
C(6*A*)—C(2*A*)—S(1*A*)	123.1 (4)	C(14*A*)—C(9*A*)—N(3*A*)	119.6 (4)
N(3*A*)—C(2*A*)—S(1*A*)	111.2 (4)	C(9*A*)—C(10*A*)—C(11*A*)	118.6 (5)
O(1*A*)—C(4*A*)—N(3*A*)	123.5 (5)	C(14*A*)—C(13*A*)—C(12*A*)	120.4 (5)
O(1*A*)—C(4*A*)—C(5*A*)	126.4 (5)	O(2*B*)—C(7*B*)—C(6*B*)	124.7 (5)
N(3*A*)—C(4*A*)—C(5*A*)	110.0 (5)	C(10*B*)—C(9*B*)—C(14*B*)	121.0 (5)
C(4*A*)—C(5*A*)—S(1*A*)	108.8 (4)	C(9*B*)—C(10*B*)—C(11*B*)	118.7 (6)
C(2*A*)—C(6*A*)—C(8*A*)	124.1 (4)	C(12*B*)—C(11*B*)—C(10*B*)	119.9 (6)
C(2*B*)—S(1*B*)—C(5*B*)	92.2 (2)	C(2*B*)—N(3*B*)—C(4*B*)	117.3 (4)
C(9*A*)—C(14*A*)—C(13*A*)	118.8 (5)	C(2*B*)—N(3*B*)—C(9*B*)	125.0 (4)
C(12*A*)—C(11*A*)—C(10*A*)	120.7 (5)	C(4*B*)—N(3*B*)—C(9*B*)	117.5 (4)
O(3*B*)—C(7*B*)—C(6*B*)	111.8 (4)	N(3*B*)—C(2*B*)—C(6*B*)	126.3 (4)
C(16*A*)—C(15*A*)—O(3*A*)	111.0 (6)	N(3*B*)—C(2*B*)—S(1*B*)	111.4 (3)
C(2*B*)—C(6*B*)—C(7*B*)	119.0 (4)	C(6*B*)—C(2*B*)—S(1*B*)	122.3 (4)
C(8*B*)—C(6*B*)—C(7*B*)	117.5 (4)	O(1*B*)—C(4*B*)—N(3*B*)	123.1 (5)
N(2*B*)—C(8*B*)—C(6*B*)	176.4 (5)	O(1*B*)—C(4*B*)—C(5*B*)	127.0 (5)
C(10*B*)—C(9*B*)—N(3*B*)	120.6 (5)	N(3*B*)—C(4*B*)—C(5*B*)	109.9 (5)
C(14*B*)—C(9*B*)—N(3*B*)	118.4 (4)	C(4*B*)—C(5*B*)—S(1*B*)	109.0 (4)
C(11*A*)—C(12*A*)—C(13*A*)	119.8 (5)	O(2*B*)—C(7*B*)—O(3*B*)	123.5 (5)
C(2*B*)—C(6*B*)—C(8*B*)	123.5 (4)	C(13*B*)—C(12*B*)—C(11*B*)	120.6 (6)
C(7*B*)—O(3*B*)—C(15*B*)	115.9 (4)	C(12*B*)—C(13*B*)—C(14*B*)	120.8 (6)
C(2*A*)—C(6*A*)—C(7*A*)	119.5 (5)	C(13*B*)—C(14*B*)—C(9*B*)	119.0 (5)
C(8*A*)—C(6*A*)—C(7*A*)	116.3 (5)	O(3*B*)—C(15*B*)—C(16*B*)	108.2 (5)

Refinement was carried out on F^2 for all reflections except for two with very negative F^2 or those flagged for potential systematic errors.

Data collection: *XSCANS* (Siemens, 1992). Cell refinement: *SHELXTL-Plus* (Sheldrick, 1991). Data reduction: *SHELXTL-Plus*. Program(s) used to solve structure: *SHELXTL-Plus*. Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *SHELXTL-Plus*. Software used to prepare material for publication: *SHELXL93* and *SHELXTL-Plus*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: SZ1026). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Tris(*n*-propyl)phosphine and Tris(isopropyl)phosphine

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Abstract

Single crystals of the low-melting title compound, tris(*n*-propyl)phosphine, $C_9H_{21}P$, (1), and its isomer, tris(isopropyl)phosphine, (2), were grown *in situ* in