

O(4)	0.5840 (4)	0.0378 (1)	-0.107 (1)	4.2 (2)
O(5)	0.7566 (5)	0.2596 (1)	0.308 (1)	3.5 (2)
O(6)	0.5722 (4)	0.2487 (1)	0.511 (1)	3.5 (2)

Table 2. Selected geometric parameters (Å, °)

C(1)—C(2)	1.398 (7)	C(10)—O(2)	1.432 (7)
C(1)—C(6)	1.379 (7)	C(11)—C(12)	1.380 (8)
C(1)—C(7)	1.471 (7)	C(11)—C(16)	1.389 (7)
C(2)—C(3)	1.380 (7)	C(12)—C(13)	1.376 (6)
C(3)—C(4)	1.390 (6)	C(13)—C(14)	1.409 (7)
C(3)—O(1)	1.377 (6)	C(13)—O(3)	1.360 (7)
C(4)—C(5)	1.394 (7)	C(14)—C(15)	1.380 (8)
C(4)—O(2)	1.362 (6)	C(14)—O(4)	1.368 (6)
C(5)—C(6)	1.385 (7)	C(15)—C(16)	1.384 (7)
C(7)—C(8)	1.337 (7)	C(17)—O(3)	1.412 (7)
C(8)—C(11)	1.486 (7)	C(18)—O(4)	1.434 (7)
C(8)—C(19)	1.505 (8)	C(19)—O(5)	1.209 (6)
C(9)—O(1)	1.405 (7)	C(19)—O(6)	1.321 (6)
C(1)—C(7)—C(8)	128.6 (5)	C(8)—C(19)—O(6)	113.0 (5)
C(2)—C(3)—O(1)	124.7 (4)	O(5)—C(19)—O(6)	123.2 (5)
C(5)—C(4)—O(2)	125.3 (5)	C(3)—O(1)—C(9)	116.8 (4)
C(12)—C(13)—O(3)	126.1 (5)	C(4)—O(2)—C(10)	117.4 (5)
C(15)—C(14)—O(4)	125.8 (5)	C(13)—O(3)—C(17)	118.3 (4)
C(8)—C(19)—O(5)	123.8 (5)	C(14)—O(4)—C(18)	116.5 (5)
C(1)—C(7)—C(8)—C(11)		-175.9 (5)	
C(1)—C(7)—C(8)—C(19)		3.6 (9)	
C(7)—C(8)—C(19)—O(5)		-110.5 (6)	

D—H...A	D...A	D—H...A
O(6)—H(O6)...O(5 ⁱ)	2.659 (5)	153 (7)

Symmetry code: (i) $\frac{2}{3} - x, y, \frac{1}{3} + z$.

The collection of the data was extended to include reflections of the type $h\bar{k}l$. A small number of reflections were affected by a minor contribution from a satellite crystal (usually this was not the case for both a reflection of the type hkl and the corresponding reflection of the type $h\bar{k}l$). The affected reflections were omitted from the data set and average F values were calculated and used in the structure analysis.

Data collection: *TEXSAN* (Molecular Structure Corporation, 1985). Cell refinement: *TEXSAN*. Data reduction: *TEXSAN*. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *TEXSAN*. Molecular graphics: *TEXSAN*. Software used to prepare material for publication: *TEXSAN*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CR1190). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2-[2-(3,4-Dichlorophenyl)vinyl]benzo-[d]thiazole

JIAN YANG

Department of Chemistry, University of Saskatchewan, Saskatoon, Saskatchewan, Canada S7N 5C9

PRAVEEN KUMAR AND JONATHAN R. DIMMOCK

College of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, Saskatchewan, Canada S7N 5C9

J. WILSON QUAIL

Department of Chemistry, University of Saskatchewan, Saskatoon, Saskatchewan, Canada S7N 5C9

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Abstract

The title compound, C₁₅H₉Cl₂NS, was synthesized by the condensation of 1-(3,4-dichlorophenyl)-4-methyl-1-penten-3-one and 2-aminothiophenol. The title compound is essentially planar in the solid state. The C=C double bond has the *E* configuration.

Comment

The synthesis of the title compound, (III), was unexpected and arose presumably by initial formation of an anil between 1-(3,4-dichlorophenyl)-4-methyl-1-penten-3-one, (I), and 2-aminothiophenol, (II), followed by attack on the carbimino C atom by the S atom leading to the extrusion of the isopropyl group and ring closure forming a benzothiazole. Alternatively, attack by the S atom on the carbonyl C atom of (I) could lead to an intermediate, the amino group of which subsequently forms a bond with this C atom, leading to ring closure and the elimination of the isopropyl group.

Data collection

Enraf-Nonius CAD-4 diffractometer	$R_{\text{int}} = 0.021$
$\omega/2\theta$ scans	$\theta_{\text{max}} = 24.92^\circ$
Absorption correction: none	$h = -7 \rightarrow 7$
2570 measured reflections	$k = 0 \rightarrow 17$
2281 independent reflections	$l = 0 \rightarrow 17$
1677 observed reflections [$I > \sigma(I)$]	3 standard reflections frequency: 120 min intensity decay: none

Refinement

Refinement on F	$\Delta\rho_{\text{max}} = 0.33 \text{ e } \text{\AA}^{-3}$
$R = 0.049$	$\Delta\rho_{\text{min}} = -0.40 \text{ e } \text{\AA}^{-3}$
$wR = 0.049$	Extinction correction: none
$S = 1.26$	Atomic scattering factors from <i>International Tables</i> for <i>X-ray Crystallography</i> (1974, Vol. IV, Table 2.2B)
1677 reflections	
172 parameters	
$w = 1/[\sigma^2(F) + 0.0005F^2]$	
$(\Delta/\sigma)_{\text{max}} < 0.001$	

C11—C3—C2	119.1 (3)	C11—C10—C15	121.2 (4)
C11—C3—C4	120.1 (3)	N—C11—C10	115.4 (3)
C2—C3—C4	120.8 (4)	N—C11—C12	124.7 (3)
C12—C4—C3	121.2 (3)	C10—C11—C12	119.9 (3)
C12—C4—C5	119.3 (3)	C11—C12—C13	118.4 (4)
C3—C4—C5	119.5 (4)	C12—C13—C14	121.4 (4)
C4—C5—C6	120.2 (4)	C13—C14—C15	120.9 (4)
C1—C6—C5	121.2 (4)	C10—C15—C14	118.1 (4)
C1—C7—C8	125.1 (4)		

The ω -scan width was $(0.80 + 0.35 \tan\theta)^\circ$ with a θ -scan rate of $0.37\text{--}2.74^\circ \text{ min}^{-1}$. The scan angle was extended 25% on each side of each peak for background measurement. All H atoms were placed in calculated positions on the corresponding C atoms (C—H = 1.00 Å) and were not refined. The U_{iso} of each H atom was assigned as equal to the U_{eq} of the attached C atom plus 0.01 \AA^2 . Refinement was by full-matrix least-squares methods.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1988). Cell refinement: *CAD-4 Software*. Data reduction: *NRCVAX DATRD2* (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to solve structure: *NRCVAX SOLVER*. Program(s) used to refine structure: *NRCVAX LSTSQ*. Molecular graphics: *NRCVAX, ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *NRCVAX TABLES* and *UTILITY*.

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \cdot a_j$$

	x	y	z	U_{eq}
C11	0.16566 (17)	0.13504 (8)	0.06737 (7)	0.0353 (6)
C12	0.62247 (16)	0.04523 (8)	0.10471 (7)	0.0297 (5)
S	-0.28655 (16)	0.17337 (7)	0.57166 (7)	0.0248 (5)
N	0.0478 (5)	0.1134 (2)	0.6672 (2)	0.023 (2)
C1	0.1962 (6)	0.1037 (3)	0.3411 (3)	0.022 (2)
C2	0.1254 (6)	0.1243 (3)	0.2508 (3)	0.023 (2)
C3	0.2554 (6)	0.1056 (3)	0.1785 (3)	0.023 (2)
C4	0.4564 (6)	0.0666 (3)	0.1943 (3)	0.022 (2)
C5	0.5275 (6)	0.0448 (3)	0.2834 (3)	0.022 (2)
C6	0.3999 (6)	0.0632 (3)	0.3556 (3)	0.023 (2)
C7	0.0564 (6)	0.1244 (3)	0.4168 (3)	0.023 (2)
C8	0.1069 (6)	0.1099 (3)	0.5054 (3)	0.026 (2)
C9	-0.0237 (6)	0.1283 (3)	0.5833 (3)	0.023 (2)
C10	-0.2991 (6)	0.1714 (3)	0.6908 (3)	0.022 (2)
C11	-0.1039 (6)	0.1374 (3)	0.7295 (3)	0.020 (2)
C12	-0.0752 (6)	0.1280 (3)	0.8252 (3)	0.025 (2)
C13	-0.2421 (7)	0.1544 (3)	0.8794 (3)	0.028 (2)
C14	-0.4359 (6)	0.1875 (3)	0.8406 (3)	0.025 (2)
C15	-0.4676 (7)	0.1964 (3)	0.7460 (3)	0.026 (2)

Table 2. Selected geometric parameters (\AA , $^\circ$)

C11—C3	1.737 (4)	C4—C5	1.386 (5)
C12—C4	1.730 (4)	C5—C6	1.373 (6)
S—C9	1.760 (4)	C7—C8	1.330 (6)
S—C10	1.739 (4)	C8—C9	1.450 (6)
N—C9	1.297 (5)	C10—C11	1.402 (5)
N—C11	1.384 (5)	C10—C15	1.399 (6)
C1—C2	1.397 (6)	C11—C12	1.401 (5)
C1—C6	1.402 (5)	C12—C13	1.388 (6)
C1—C7	1.466 (6)	C13—C14	1.390 (6)
C2—C3	1.385 (6)	C14—C15	1.387 (6)
C3—C4	1.380 (5)		
C9—S—C10	89.1 (2)	C7—C8—C9	127.9 (4)
C9—N—C11	111.2 (3)	S—C9—N	115.2 (3)
C2—C1—C6	118.1 (4)	S—C9—C8	123.1 (3)
C2—C1—C7	119.4 (3)	N—C9—C8	121.7 (3)
C6—C1—C7	122.5 (3)	S—C10—C11	109.0 (3)
C1—C2—C3	120.3 (4)	S—C10—C15	129.7 (3)

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: PT1025). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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