

Li-Li Bao, Zhi-Jin Fan,* Hai-Bin Song and Kai-Sheng Nie

State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, People's Republic of China

Correspondence e-mail: fanzj@nankai.edu.cn

Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.036
 wR factor = 0.103
Data-to-parameter ratio = 12.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.***N*-Phenyl-*N'*-(1,3-thiazol-2-yl)-1,2,3-benzothiadiazole-7-carboxamide**

The title compound, $\text{C}_{16}\text{H}_{11}\text{N}_5\text{S}_2$, is a potent new plant elicitor (activator). The benzothiadiazole ring system is essentially planar and forms a dihedral angle of $15.76(4)^\circ$ with the thiazole ring. An $\text{N}-\text{H}\cdots\text{N}$ intramolecular hydrogen-bonding interaction is present.

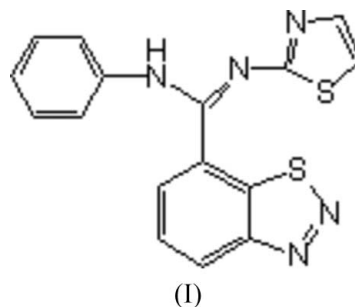
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Comment

Benzothiadiazole derivatives are important plant elicitors (Fan *et al.*, 2005), which can induce systemic acquired resistance in the treated plants against pathogen attack. Similarly, carboxamide derivatives can also induce systemic acquired resistance in some plants (Kunz & Schurter, 1995). In view of this property and our interest in the chemistry of benzothiadiazoles, we have attempted to synthesize a series of carboxamide derivatives, some of which have comparatively high activity. The crystal structure determination of the title compound, (I), was undertaken to investigate the relationship between structure and induction of systemic acquired resistance.



The molecular structure of (I) is shown in Fig. 1. X-ray analysis reveals that the benzothiadiazole ring system is essentially planar, with maximum deviations from the mean plane ranging from $-0.052(1)$ to $0.051(2)$ Å, and not coplanar with the thiazole ring, the dihedral angle between them being $15.76(4)^\circ$. The C8–C13 phenyl ring is twisted by $54.79(5)^\circ$ with respect to the mean plane of the benzothiadiazole system.

An $\text{N}-\text{H}\cdots\text{N}$ intramolecular hydrogen-bonded interaction (Table 2) is present, stabilizing the molecular structure.

Experimental

Compound (I) was prepared according to the reported procedure of Gönczi *et al.* (1981). Single crystals suitable for X-ray diffraction were obtained by recrystallization from a mixture of ethyl acetate and petroleum ether (1:6 *v/v*).

Crystal data

$C_{16}H_{11}N_5S_2$
 $M_r = 337.42$
 Triclinic, $P\bar{1}$
 $a = 8.6537$ (18) Å
 $b = 8.8624$ (18) Å
 $c = 10.474$ (2) Å
 $\alpha = 81.713$ (3)°
 $\beta = 74.134$ (3)°
 $\gamma = 84.719$ (3)°
 $V = 763.4$ (3) Å³

$Z = 2$
 $D_x = 1.468$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 1970 reflections
 $\theta = 2.3$ – 26.3 °
 $\mu = 0.35$ mm⁻¹
 $T = 294$ (2) K
 Prism, colourless
 0.22 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.910$, $T_{max} = 0.965$
 3909 measured reflections

2678 independent reflections
 2075 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.018$
 $\theta_{max} = 25.0$ °
 $h = -10 \rightarrow 7$
 $k = -10 \rightarrow 10$
 $l = -11 \rightarrow 12$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.103$
 $S = 1.02$
 2678 reflections
 212 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.161P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.15$ e Å⁻³
 $\Delta\rho_{min} = -0.26$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

N3—C7	1.346 (2)	C6—C7	1.486 (3)
N4—C14	1.368 (2)	C15—C16	1.337 (3)
C1—S1—N1	92.16 (11)	C7—N4—C14	122.06 (17)
C7—N3—C8	128.41 (16)	C2—C1—C6—C7	176.29 (17)
N1—N2—C2—C3	176.2 (2)		
S1—C1—C6—C5	173.33 (16)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3A \cdots N5	0.89 (1)	1.99 (1)	2.714 (2)	137 (1)

The H atom attached to the N atom was found in a difference Fourier map and refined freely. H atoms attached to C atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

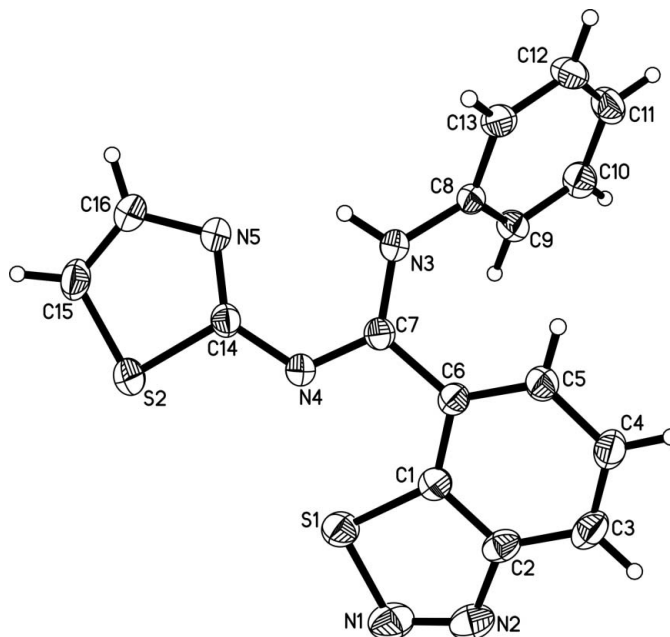


Figure 1

A view of (I), with displacement ellipsoids drawn at the 30% probability level.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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