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N-(4-Methylpyrimidin-2-yl)bis(1,2,3-benzothiadiazole-7-carbonyl)amine

Ying-Wei Ai,[a] Yong-Gang Zhang,[b] Feng-Li Liu,[b] Hai-Bin Song[b] and Zhi-Jin Fan[b,c]*

[a]Key Laboratory of Bio-resources and Eco-environment (Ministry of Education), College of Life Sciences, Sichuan University, Chengdu, Sichuan 610064, People's Republic of China, [b]State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, People's Republic of China, and [c]Key Laboratory of Pesticide Chemistry and Application Technology of the Ministry of Agriculture, Beijing 100094, People's Republic of China

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

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.107
Data-to-parameter ratio = 13.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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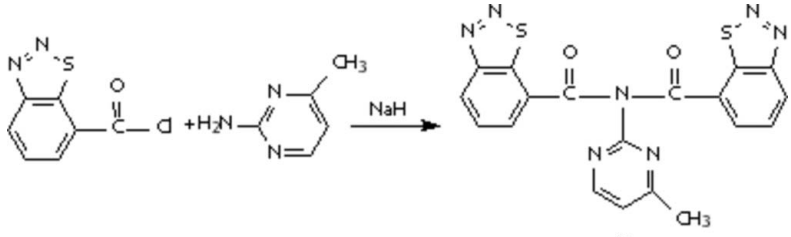
The title compound, $C_{19}H_{11}N_7O_2S_2$, was synthesized as a potential new plant elicitor, by reaction of 2-amino-4-methylpyrimidine with 1,2,3-benzothiadiazole-7-carbonyl chloride. There are two crystallographically independent molecules in the asymmetric unit. In the crystal structure, the molecules are linked by a weak C—H···N hydrogen-bonding interaction.

Comment

Plant elicitors (activators) are a new class of agrochemicals with a new mode of action which have attracted much interest in China (Gozzo, 2003; Fan, Liu & Liu, 2005; Bao, Liu & Fan, 2005). Our research team has synthesized a series of benzothiadiazole derivatives (Liu, 2005), some of which can induce in tobacco a comparatively high resistance to tobacco mosaic virus (TMV). In an investigation of the quantitative structure–activity relationship (QSAR) of this new type of pesticides, we have recently reported the structures of some of them (Bao, Fan *et al.*, 2005; Ai *et al.*, 2005; Liu *et al.*, 2005; Zhao *et al.*, 2006). We report here the crystal structure of the title compound, (I), which represents an example of an *N*-substituted carboximide derivative of benzothiadiazole.



(I)

The asymmetric unit of (I) (Fig. 1) contains two crystallographically independent molecules, *A* (atoms S1/S2/O1/O2/N1–N7/C1–C19) and *B* (atoms S3/S4/O3/O4/N8–N14/C20–C38). The bond lengths and angles in (I) are normal, and the values for the two independent molecules agree well with each other (Table 1). In both molecules, the two benzothiadiazole ring systems are essentially planar, forming dihedral angles of 77.5 (1) and 77.8 (1)° in molecules *A* and *B*, respectively. The pyrimidine rings are also essentially planar, with a maximum deviation from planarity of 0.027 (4) Å for atom C4. The dihedral angles formed by the pyrimidine rings and the benzothiadiazole rings are 61.6 (1) and 75.2 (1)° in molecule *A*, and 66.9 (1) and 74.7 (1)° in molecule *B*.

The crystal structure of (I) is stabilized by a weak C—H···N hydrogen bond (Table 2).

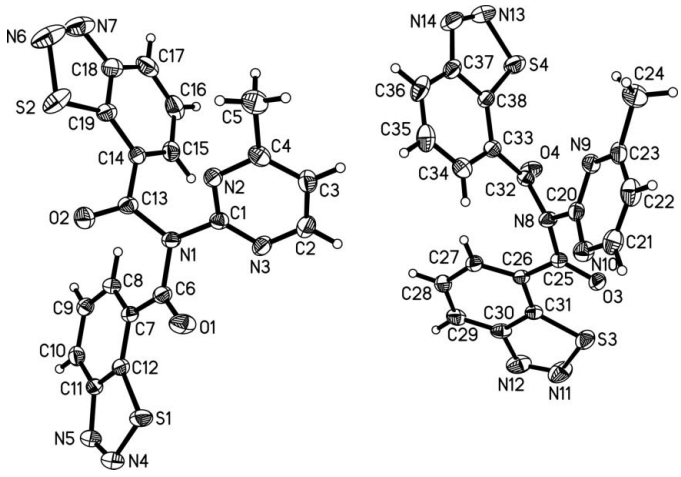


Figure 1
A view of the asymmetric unit of the title compound, with displacement ellipsoids drawn at the 30% probability level.

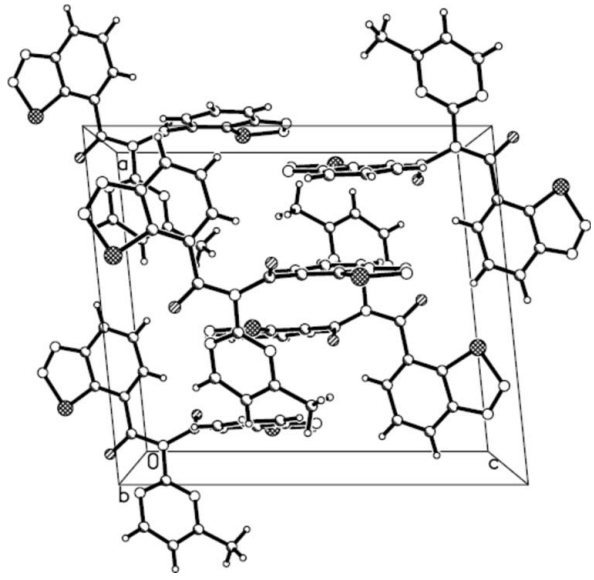


Figure 2
The crystal packing of the title compound, viewed along the *b* axis.

Experimental

The title compound was synthesized by the reaction of 2-amino-4-methylpyrimidine with 1,2,3-benzothiadiazole-7-carboxylic acid chloride according to the reported precedure of Fan, Liu, Liu *et al.* (2005). Light-yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a petroleum ether–ethyl acetate solution (3:1 *v/v*) at room temperature.

Crystal data

$C_{19}H_{11}N_7O_2S_2$
M_r = 433.47
Monoclinic, $P2_1$
a = 11.689 (3) Å
b = 12.283 (3) Å
c = 13.223 (3) Å
β = 95.771 (4)°
V = 1889.0 (8) Å^3
Z = 4
D_x = 1.524 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3817 reflections
θ = 2.4–26.1°
μ = 0.32 mm^{-1}
T = 293 (2) K
Prism, light-yellow
0.28 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.902, T_{max} = 0.945
11005 measured reflections
7122 independent reflections
5141 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 26.4°
$h = -12 \rightarrow 14$
$k = -12 \rightarrow 15$
$l = -16 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.107
S = 1.03
7122 reflections
543 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.0505P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack (1983), with 4042 Friedel pairs
Flack parameter: −0.03 (7)

Table 1
Selected geometric parameters (Å, °).

S1—C12	1.696 (3)	N4—N5	1.276 (4)
S1—N4	1.705 (3)	N5—C11	1.380 (4)
S2—N6	1.708 (4)	N6—N7	1.273 (6)
S2—C19	1.711 (4)	N7—C18	1.397 (6)
S3—C31	1.702 (4)	N8—C32	1.423 (4)
S3—N11	1.713 (4)	N8—C25	1.428 (4)
S4—C38	1.703 (4)	N8—C20	1.434 (4)
S4—N13	1.708 (4)	N9—C20	1.323 (4)
N1—C13	1.414 (4)	N9—C23	1.354 (5)
N1—C6	1.426 (4)	N10—C20	1.313 (5)
N1—C1	1.429 (4)	N10—C21	1.346 (5)
N2—C1	1.329 (4)	N11—N12	1.257 (5)
N2—C4	1.345 (4)	N12—C30	1.386 (5)
N3—C1	1.311 (4)	N13—N14	1.268 (5)
N3—C2	1.329 (5)	N14—C37	1.376 (5)
C12—S1—N4	91.79 (17)	N7—N6—S2	112.5 (3)
N6—S2—C19	92.4 (2)	N6—N7—C18	113.8 (4)
C31—S3—N11	92.06 (18)	C32—N8—C25	119.0 (3)
C38—S4—N13	91.7 (2)	C32—N8—C20	117.2 (2)
C13—N1—C6	119.8 (3)	C25—N8—C20	119.3 (3)
C13—N1—C1	117.6 (2)	C20—N9—C23	114.7 (3)
C6—N1—C1	117.6 (3)	C20—N10—C21	114.5 (3)
C1—N2—C4	115.3 (3)	N12—N11—S3	112.7 (3)
C1—N3—C2	114.1 (3)	N11—N12—C30	114.6 (3)
N5—N4—S1	113.8 (2)	N14—N13—S4	112.8 (3)
N4—N5—C11	112.6 (3)	N13—N14—C37	113.5 (4)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···N1	0.93	2.62	2.930 (4)	100

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.96 Å, and U_{iso}(H) = 1.2 (aromatic H atoms) or 1.5 (methyl H atoms) times U_{eq}(C).

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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