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Phenyl *N*-(1,3-thiazol-2-yl)carbamateJian-Guo Tang,^a Yong-Zhong Wu,^b Sheng Bi,^a Guo-Hua Zhang^a and Cheng Guo^{a*}

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Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.050; wR factor = 0.160; data-to-parameter ratio = 13.8.

In the title compound, $\text{C}_{10}\text{H}_8\text{N}_2\text{O}_2\text{S}$, the planes of the aromatic rings are oriented at a dihedral angle of $66.69(3)^\circ$. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{O}$ interactions link the molecules into a two-dimensional network, forming $R_2^2(8)$ ring motifs. $\pi-\pi$ contacts between the thiazole rings [centroid-centroid distance = $3.535(1)$ Å] may further stabilize the structure. A weak $\text{C}-\text{H}\cdots\pi$ interaction is also found.

Related literature

For a related structure, see: Araujo *et al.* (2006). For bond-length data, see: Allen *et al.* (1987). For ring-motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$\text{C}_{10}\text{H}_8\text{N}_2\text{O}_2\text{S}$
 $M_r = 220.24$
 Monoclinic, $P2_1/c$
 $a = 5.6430(11)$ Å
 $b = 7.3910(15)$ Å

$c = 25.134(5)$ Å
 $\beta = 91.21(3)^\circ$
 $V = 1048.0(4)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.29$ mm⁻¹
 $T = 294$ K

0.30 × 0.20 × 0.10 mm

Data collection

Enraf-Nonius CAD-4 diffractometer
 Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.918$, $T_{\max} = 0.972$
 2084 measured reflections

1880 independent reflections
 1346 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 3 standard reflections
 frequency: 120 min
 intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.160$
 $S = 1.00$
 1880 reflections

136 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.28$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{N2}^i$	0.86	2.01	2.864 (4)	171
$\text{C3}-\text{H3A}\cdots\text{O2}^{ii}$	0.93	2.46	3.335 (4)	156
$\text{C5}-\text{H5A}\cdots\text{Cg2}^{iii}$	0.93	2.98	3.736 (3)	139

Symmetry codes: (i) $-x, -y + 2, -z$; (ii) $x - 1, y, z$; (iii) $x, y + 1, z$. Cg2 is the centroid of the S/N2/C8-C10 ring.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2701).

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supplementary materials

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Phenyl *N*-(1,3-thiazol-2-yl)carbamate

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Comment

Some derivatives of phenol are important chemical materials. We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (C1-C6) and B (S/N2/C8-C10) are, of course, planar and they are oriented at a dihedral angle of 66.69 (3)°. Atoms O1, O2, N1, C4, C7, H1A, H9A and H10B are 0.118 (3), -0.063 (3), 0.028 (3), 0.172 (3), 0.023 (3), 0.051 (3), 0.002 (3) and -0.002 (3) Å away from the plane of ring B, respectively.

In the crystal structure, intermolecular N-H...N and C-H...O interactions (Table 1) link the molecules into a two-dimensional network forming $R_2^2(8)$ ring motifs (Bernstein *et al.*, 1995) (Fig. 2), in which they may be effective in the stabilization of the structure. The π - π contact between the thiazole rings, Cg2—Cg2¹, [symmetry code: (i) 1 - x, -y, -z, where Cg2 is centroid of the ring B (S/N2/C8-C10)] may further stabilize the structure, with centroid-centroid distance of 3.535 (1) Å. There also exists a weak C—H... π interaction (Table 1).

Experimental

For the preparation of the title compound, phenyl chloroformate (1.0 ml) was added slowly to a cold solution of thiazol-2-amine (1.0 g) and triethylamine (0.8 ml) in methylene chloride (10 ml) at 273 K. The mixture was then warmed and stirred for 1 h at room temperature. Then, it was washed with water (20 ml), dried and concentrated to give the title compound (yield; 1.3 g) (Araujo *et al.*, 2006). Crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution.

Refinement

H atoms were positioned geometrically, with N-H = 0.86 Å (for NH) and C-H = 0.93 Å for aromatic H and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$.

Figures

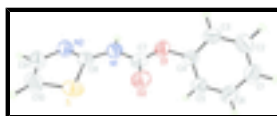


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

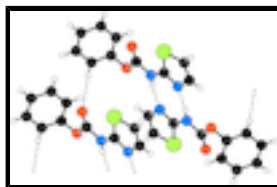


Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

Phenyl *N*-(1,3-thiazol-2-yl)carbamate

Crystal data

C₁₀H₈N₂O₂S

M_r = 220.24

Monoclinic, *P*2₁/*c*

Hall symbol: -*P* 2ybc

a = 5.6430 (11) Å

b = 7.3910 (15) Å

c = 25.134 (5) Å

β = 91.21 (3)°

V = 1048.0 (4) Å³

Z = 4

*F*₀₀₀ = 456

D_x = 1.396 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 25 reflections

θ = 9–13°

μ = 0.29 mm⁻¹

T = 294 K

Block, colorless

0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 294 K

ω/2θ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

*T*_{min} = 0.918, *T*_{max} = 0.972

2084 measured reflections

1880 independent reflections

1346 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.027

θ_{max} = 25.3°

θ_{min} = 1.6°

h = 0→6

k = 0→8

l = -30→30

3 standard reflections

every 120 min

intensity decay: 1%

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.050

wR(*F*²) = 0.160

S = 1.00

1880 reflections

136 parameters

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 1.2P]$$

where *P* = (*F*_o² + 2*F*_c²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 0.23 e Å⁻³

Δρ_{min} = -0.28 e Å⁻³

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S	0.50888 (16)	0.91653 (14)	0.09893 (4)	0.0578 (3)
O1	-0.0749 (4)	1.3216 (4)	0.10691 (9)	0.0584 (7)
O2	0.2490 (4)	1.1925 (4)	0.14685 (10)	0.0604 (7)
N1	0.0988 (5)	1.0912 (4)	0.06773 (11)	0.0522 (8)
H1A	-0.0156	1.1050	0.0449	0.063*
N2	0.2450 (5)	0.8574 (4)	0.01638 (11)	0.0535 (8)
C1	-0.1494 (7)	1.7169 (6)	0.22167 (16)	0.0653 (11)
H1B	-0.1690	1.8072	0.2470	0.078*
C2	-0.3070 (7)	1.5775 (6)	0.21820 (16)	0.0700 (12)
H2B	-0.4336	1.5728	0.2413	0.084*
C3	-0.2801 (6)	1.4432 (5)	0.18072 (15)	0.0583 (10)
H3A	-0.3880	1.3484	0.1781	0.070*
C4	-0.0921 (6)	1.4522 (5)	0.14755 (13)	0.0476 (8)
C5	0.0675 (7)	1.5907 (5)	0.15058 (15)	0.0592 (10)
H5A	0.1945	1.5943	0.1276	0.071*
C6	0.0395 (8)	1.7244 (6)	0.18762 (16)	0.0666 (11)
H6A	0.1470	1.8196	0.1899	0.080*
C7	0.1061 (6)	1.2010 (5)	0.11072 (14)	0.0494 (9)
C8	0.2638 (6)	0.9587 (5)	0.05834 (13)	0.0446 (8)
C9	0.4328 (7)	0.7386 (5)	0.01506 (16)	0.0617 (10)
H9A	0.4494	0.6552	-0.0123	0.074*
C10	0.5867 (7)	0.7498 (6)	0.05473 (17)	0.0651 (11)
H10B	0.7206	0.6772	0.0585	0.078*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0439 (5)	0.0727 (7)	0.0563 (6)	-0.0038 (5)	-0.0113 (4)	0.0105 (5)
O1	0.0530 (14)	0.0639 (17)	0.0574 (15)	0.0055 (13)	-0.0160 (12)	-0.0165 (13)
O2	0.0554 (15)	0.0714 (18)	0.0536 (15)	-0.0004 (13)	-0.0156 (12)	-0.0085 (13)
N1	0.0431 (15)	0.0635 (19)	0.0493 (16)	0.0000 (15)	-0.0130 (13)	-0.0135 (15)
N2	0.0532 (17)	0.0526 (17)	0.0542 (17)	0.0043 (15)	-0.0076 (14)	-0.0044 (15)

supplementary materials

C1	0.066 (3)	0.072 (3)	0.058 (2)	0.010 (2)	-0.0082 (19)	-0.014 (2)
C2	0.053 (2)	0.094 (3)	0.063 (2)	0.003 (2)	0.0069 (19)	-0.007 (2)
C3	0.0443 (19)	0.067 (3)	0.064 (2)	-0.0096 (18)	-0.0019 (17)	-0.002 (2)
C4	0.0482 (19)	0.049 (2)	0.0453 (19)	-0.0013 (16)	-0.0090 (15)	-0.0020 (16)
C5	0.057 (2)	0.065 (3)	0.055 (2)	-0.011 (2)	0.0101 (17)	-0.0055 (19)
C6	0.072 (3)	0.062 (2)	0.066 (3)	-0.016 (2)	-0.003 (2)	-0.009 (2)
C7	0.0454 (19)	0.052 (2)	0.051 (2)	-0.0129 (17)	-0.0057 (16)	-0.0003 (17)
C8	0.0433 (18)	0.0499 (19)	0.0403 (18)	-0.0062 (16)	-0.0056 (14)	0.0051 (15)
C9	0.068 (2)	0.056 (2)	0.062 (2)	0.007 (2)	-0.0016 (19)	-0.0001 (19)
C10	0.054 (2)	0.061 (2)	0.080 (3)	0.0108 (19)	0.001 (2)	0.017 (2)

Geometric parameters (Å, °)

S—C10	1.722 (4)	C1—H1B	0.9300
S—C8	1.729 (3)	C2—C3	1.379 (5)
O1—C4	1.410 (4)	C2—H2B	0.9300
O1—C7	1.358 (4)	C3—C4	1.364 (5)
O2—C7	1.203 (4)	C3—H3A	0.9300
N1—C7	1.351 (4)	C4—C5	1.365 (5)
N1—C8	1.375 (4)	C5—C6	1.369 (5)
N1—H1A	0.8600	C5—H5A	0.9300
N2—C8	1.296 (4)	C6—H6A	0.9300
N2—C9	1.377 (5)	C9—C10	1.311 (6)
C1—C2	1.363 (6)	C9—H9A	0.9300
C1—C6	1.382 (6)	C10—H10B	0.9300
C10—S—C8	87.71 (18)	C4—C5—C6	119.6 (4)
C7—O1—C4	117.5 (2)	C4—C5—H5A	120.2
C7—N1—C8	123.7 (3)	C6—C5—H5A	120.2
C7—N1—H1A	118.1	C5—C6—C1	119.6 (4)
C8—N1—H1A	118.1	C5—C6—H6A	120.2
C2—C1—C6	120.1 (4)	C1—C6—H6A	120.2
C2—C1—H1B	120.0	O2—C7—N1	125.5 (3)
C6—C1—H1B	120.0	O2—C7—O1	125.4 (3)
C8—N2—C9	109.8 (3)	N1—C7—O1	109.1 (3)
C1—C2—C3	120.4 (4)	N2—C8—N1	120.5 (3)
C1—C2—H2B	119.8	N2—C8—S	115.2 (3)
C3—C2—H2B	119.8	N1—C8—S	124.3 (2)
C4—C3—C2	118.7 (4)	C10—C9—N2	116.0 (4)
C4—C3—H3A	120.6	C10—C9—H9A	122.0
C2—C3—H3A	120.6	N2—C9—H9A	122.0
C3—C4—C5	121.5 (3)	C9—C10—S	111.2 (3)
C3—C4—O1	118.4 (3)	C9—C10—H10B	124.4
C5—C4—O1	119.9 (3)	S—C10—H10B	124.4
C6—C1—C2—C3	-0.2 (6)	C4—O1—C7—O2	2.5 (5)
C1—C2—C3—C4	0.5 (6)	C4—O1—C7—N1	-178.0 (3)
C2—C3—C4—C5	-0.3 (6)	C9—N2—C8—N1	178.6 (3)
C2—C3—C4—O1	-175.6 (3)	C9—N2—C8—S	-0.2 (4)
C7—O1—C4—C3	-112.5 (4)	C7—N1—C8—N2	179.5 (3)
C7—O1—C4—C5	72.1 (4)	C7—N1—C8—S	-1.8 (5)

C3—C4—C5—C6	-0.1 (6)	C10—S—C8—N2	0.1 (3)
O1—C4—C5—C6	175.2 (3)	C10—S—C8—N1	-178.6 (3)
C4—C5—C6—C1	0.3 (6)	C8—N2—C9—C10	0.2 (5)
C2—C1—C6—C5	-0.2 (6)	N2—C9—C10—S	-0.2 (5)
C8—N1—C7—O2	-3.3 (6)	C8—S—C10—C9	0.0 (3)
C8—N1—C7—O1	177.2 (3)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1A...N2 ⁱ	0.86	2.01	2.864 (4)	171
C3—H3A...O2 ⁱⁱ	0.93	2.46	3.335 (4)	156
C5—H5A...Cg2 ⁱⁱⁱ	0.93	2.98	3.736 (3)	139

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $x-1, y, z$; (iii) $x, y+1, z$.

Fig. 1

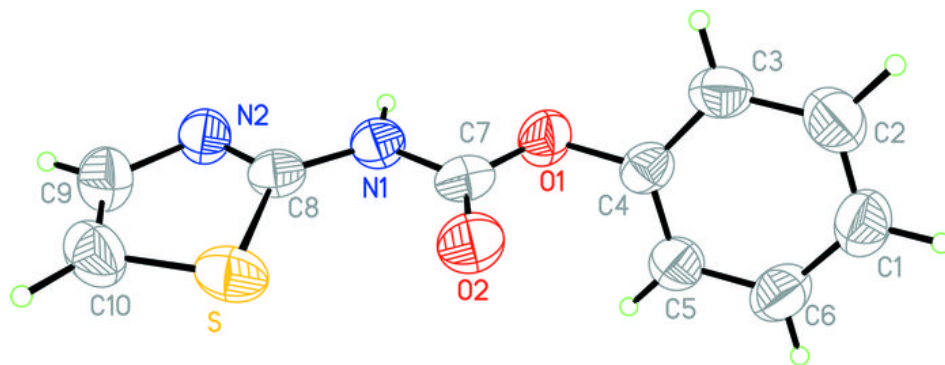


Fig. 2

