Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

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

**Jian-Guo Tang,[a] Yong-Zhong Wu,[b] Sheng Bi,[a] Guo-Hua Zhang[a] and Cheng Guo[a]***

[a]College of Science, Nanjing University of Technology, Xinmofan Road No. 5 Nanjing, Nanjing 210009, People's Republic of China, and [b]Department of Applied Chemistry, Nanjing College of Chemical Technology, Geguan Road No. 625 Dachang District Nanjing, Nanjing 210048, People's Republic of China
Correspondence e-mail: guocheng@njut.edu.cn

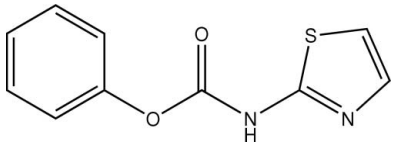
Received 25 May 2009; accepted 27 May 2009

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

In the title compound, $C_{10}H_8N_2O_2S$, the planes of the aromatic rings are oriented at a dihedral angle of 66.69 (3)°. In the crystal structure, intermolecular N—H···N and C—H···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 C—H···$\pi$ 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*

$C_{10}H_8N_2O_2S$
$M_r$ = 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)°
$V$ = 1048.0 (4) Å$^3$
$Z$ = 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: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.918, $T_{max}$ = 0.972
2084 measured reflections
1880 independent reflections
1346 reflections with $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···N2$^{i}$ | 0.86 | 2.01 | 2.864 (4) | 171 |
| C3—H3$A$···O2$^{ii}$ | 0.93 | 2.46 | 3.335 (4) | 156 |
| C5—H5$A$···$Cg2^{iii}$ | 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*.

The authors thank the Center of Testing and Analysis, Nanjing University, for support.

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

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Araujo, M., Eduarda, M. & Norberto, F. (2006). *J. Chem. Res.* **10**, 664–667.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supplementary materials

*Acta Cryst.* (2009). E**65**, o1478 [ **doi:10.1107/S1600536809020236** ]

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

**J.-G. Tang, Y.-Z. Wu, S. Bi, G.-H. Zhang and C. Guo**

## 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—Cg2$^{i}$, [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 $U_{iso}(H) = 1.2U_{eq}(C,N)$.

## Figures

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

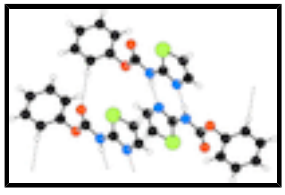


Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

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

### *Crystal data*

| | |
|---|---|
| $C_{10}H_8N_2O_2S$ | $F_{000} = 456$ |
| $M_r = 220.24$ | $D_x = 1.396$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 25 reflections |
| $a = 5.6430$ (11) Å | $\theta = 9$–13º |
| $b = 7.3910$ (15) Å | $\mu = 0.29$ mm$^{-1}$ |
| $c = 25.134$ (5) Å | $T = 294$ K |
| $\beta = 91.21$ (3)º | Block, colorless |
| $V = 1048.0$ (4) Å$^3$ | 0.30 × 0.20 × 0.10 mm |
| $Z = 4$ | |

### *Data collection*

| | |
|---|---|
| Enraf–Nonius CAD-4 diffractometer | $R_{int} = 0.027$ |
| Radiation source: fine-focus sealed tube | $\theta_{max} = 25.3$º |
| Monochromator: graphite | $\theta_{min} = 1.6$º |
| $T = 294$ K | $h = 0 \rightarrow 6$ |
| $\omega/2\theta$ scans | $k = 0 \rightarrow 8$ |
| Absorption correction: $\psi$ scan (North *et al.*, 1968) | $l = -30 \rightarrow 30$ |
| $T_{min} = 0.918$, $T_{max} = 0.972$ | 3 standard reflections |
| 2084 measured reflections | every 120 min |
| 1880 independent reflections | intensity decay: 1% |
| 1346 reflections with $I > 2\sigma(I)$ | |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.050$ | H-atom parameters constrained |
| $wR(F^2) = 0.160$ | $w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 1.2P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.00$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 1880 reflections | $\Delta\rho_{max} = 0.23$ e Å$^{-3}$ |
| 136 parameters | $\Delta\rho_{min} = -0.28$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 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, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| 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**

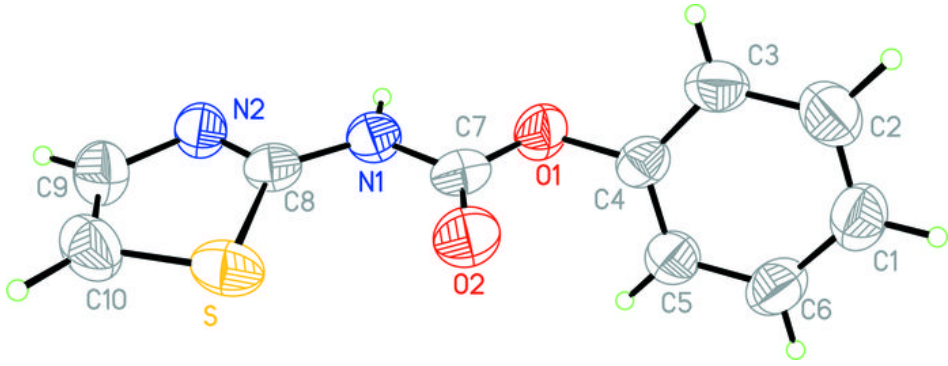


**Fig. 2**