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2-Benzoyl-*N*-phenyl-2-(1,2,4-triazol-1-yl)thioacetamide and 2-(4-methoxybenzoyl)-*N*-phenyl-2-(1,2,4-triazol-1-yl)thioacetamide

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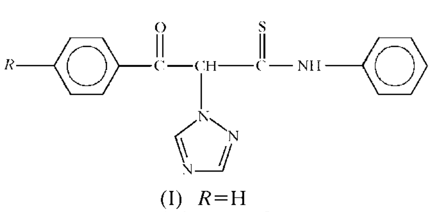
In the two title compounds, $C_{17}H_{14}N_4OS$, (I), and $C_{18}H_{16}N_4O_2S$, (II), the dihedral angles between the planes of the triazole and *N*-phenyl rings and the plane of five of the atoms that link these two rings are 63.5 (8) and 73.2 (6)° for (I), and 65.1 (1) and 72.1 (3)° for (II), respectively. There are some inter- and intramolecular interactions in the crystal structure.

Comment

Recently, compounds containing the 1*H*-1,2,4-triazole group have attracted much interest because they exhibit some fungicidal activity and plant-growth regulating activity (Xu *et al.*, 2002), and show antibacterial activity against *Puccinia recondite* and root-growth regulation for cucumber (Zhao *et al.*, 1998). In order to search for new triazole compounds with higher bioactivity, we synthesized the title compounds, (I) and (II). Their structures are described here.



(I) R=H
(II) R=MeO

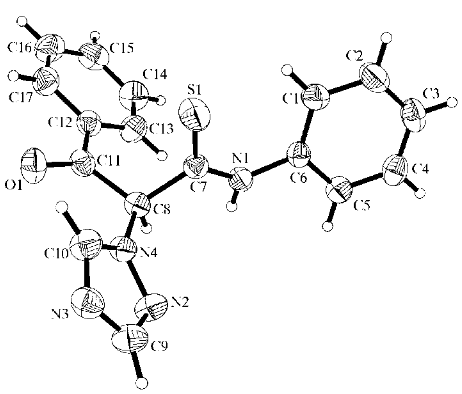


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

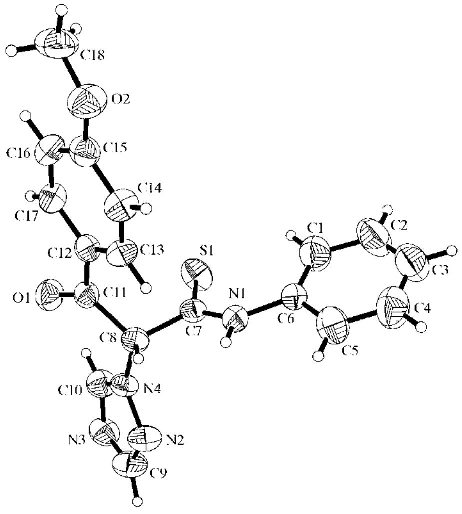


Figure 2
The structure of (II), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

In the title compounds (Figs. 1 and 2), the bond lengths and angles are generally normal in the *N*-phenyl and triazole rings (Ji *et al.*, 2002). The C═S bond length (Tables 1 and 3) in each compound is close to the typical C═S double-bond length. Atom C8 lies in the plane of the triazole ring, and atoms S1, C6, C7, C8 and N1 are coplanar (plane *p*1). The dihedral angles formed by the C1–C6 and triazole rings with *p*1 are 63.5 (8) and 73.2 (6)° for (I), and 65.1 (1) and 72.1 (3)° for (II), respectively. These values indicate that the addition of the methoxy group to the C12–C17 benzene ring has little influence on the molecular conformation. The C1—C6—N1—C7, N2—N4—C8—C7, N2—N4—C8—C11 and N4—C8—C11—C12 torsion angles are 25.3 (5), 88.5 (0), 147.4 (6) and 175.5 (6)° for (I), and 13.1 (0), 88.8 (8), 147.5 (9) and 171.3 (8)° for (II), respectively. The C14—C15—O2—C18 torsion angle is 173.0 (6)° for (II).

The most interesting structural features of the two complexes are the N—H···N intermolecular hydrogen bonds and the weak (C—H···*Y* hydrogen bonds; *Y* = O, N and S) intermolecular interactions (see Tables 2 and 4). These interactions stabilize the two structures.

Experimental

The title compounds were prepared by the reaction of α-(1,2,4-triazol-1-yl)acetophenone, phenyl isothiocynate [for (I)] or methoxyphenyl isothiocynate [for (II)], and potassium hydroxide in dimethyl sulfoxide solution. Single crystals of the title compounds suitable for X-ray measurements were obtained by recrystallization from chloroform/ethyl acetate (1:3 *v*/*v*) at room temperature.

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Compound (I)

Crystal data

$C_{17}H_{14}N_4OS$
$M_r = 322.38$
Monoclinic, $P2_1/c$
$a = 8.8060$ (18) Å
$b = 12.097$ (2) Å
$c = 14.809$ (3) Å
$\beta = 105.88$ (3)°
$V = 1517.3$ (6) Å^3
$Z = 4$

$D_x = 1.411$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
$\theta = 2$–11°
$\mu = 0.22$ mm^{-1}
$T = 293$ (2) K
Pillar, yellow
0.25 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS-IV Imaging Plate diffractometer
Oscillation frame scans
5518 measured reflections
3055 independent reflections
2314 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$

$\theta_{\max} = 26.5°$
$h = -10 \rightarrow 0$
$k = -15 \rightarrow 15$
$l = -17 \rightarrow 19$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.103$
$S = 1.09$
3055 reflections
209 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 0.2377P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.21$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0133 (17)

Table 1
Selected interatomic distances (Å) for (I).

S1—C7	1.6536 (18)	N1—C6	1.425 (2)
O1—C11	1.214 (2)	N2—C9	1.314 (2)
N1—C7	1.342 (2)	N2—N4	1.368 (2)

Table 2
Hydrogen-bonding geometry (Å, °) for (I).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N3$^{\rm i}$	0.86	2.14	2.998 (2)	174
C1—H1*B*···S1	0.93	2.67	3.248 (2)	120
C10—H10*A*···O1	0.93	2.40	2.758 (3)	103

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

Compound (II)

Crystal data

$C_{18}H_{16}N_4O_2S$
$M_r = 352.41$
Monoclinic, $P2_1/c$
$a = 9.806$ (2) Å
$b = 11.677$ (2) Å
$c = 16.002$ (5) Å
$\beta = 112.55$ (2)°
$V = 1692.2$ (7) Å^3
$Z = 4$

$D_x = 1.383$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
$\theta = 2$–11°
$\mu = 0.21$ mm^{-1}
$T = 293$ (2) K
Pillar, yellow
0.25 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS-IV Imaging Plate diffractometer
Oscillation frame scans
5351 measured reflections
3195 independent reflections
2209 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.029$

$\theta_{\max} = 25.9°$
$h = 0 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -20 \rightarrow 18$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.078$
$wR(F^2) = 0.240$
$S = 1.12$
3195 reflections
227 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1328P)^2 + 0.7232P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 1.10$ e Å^{-3}
$\Delta\rho_{\min} = -0.33$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.013 (4)

Table 3
Selected interatomic distances (Å) for (II).

S1—C7	1.653 (4)	N1—C7	1.339 (5)
O1—C11	1.217 (4)	N1—C6	1.427 (5)
O2—C15	1.379 (5)	N2—C9	1.317 (6)
O2—C18	1.389 (6)	N2—N4	1.359 (5)

Table 4
Hydrogen-bonding geometry (Å, °) for (II).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N3$^{\rm ii}$	0.86	2.22	3.076 (5)	175
C1—H1*B*···S1	0.93	2.62	3.256 (6)	126
C8—H8*A*···N3$^{\rm ii}$	0.98	2.63	3.537 (5)	154
C10—H10*A*···O1	0.93	2.42	2.811 (6)	105

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

H atoms were positioned geometrically and treated as riding on their parent C atoms, with C—H distances in the range 0.93–0.98 Å and $U_{\rm iso}$(H) values of 1.2 and 1.5 times the $U_{\rm eq}$ values of the parent atoms.

For both compounds, data collection: *R-AXIS Software* (Rigaku, 1997); cell refinement: *R-AXIS Software*; data reduction: *R-AXIS Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990*b*); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1659). Services for accessing these data are described at the back of the journal.

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