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2-Anilino-5-benzoyl-4-phenyl-1,3-thiazole

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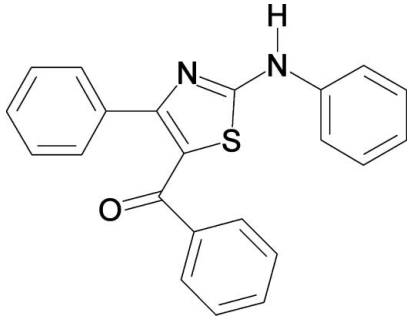
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.116; data-to-parameter ratio = 18.0.

Under basic conditions, methyl-*N*-phenylthiocarbomylphenylimidate and phenacyl bromide form the title compound, $C_{22}H_{16}N_2OS$. X-ray diffraction shows that the crystal structure can be described as consisting of pseudo-dimers resulting from intermolecular N—H···N hydrogen bonds, which are further stabilized by van der Waals interactions.

Related literature

For general background, see: Dridi *et al.* (1998); El Efrit *et al.* (1996); Gorczynski *et al.* (2004); Wipf *et al.* (2001). For structural information, see: Allen (2002); Etter *et al.* (1990); Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{22}H_{16}N_2OS$
M_r = 356.43
Monoclinic, $P2_1/n$
a = 13.163 (4) Å
b = 9.433 (4) Å
c = 14.533 (2) Å
β = 99.33 (2)°
V = 1780.7 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.16 mm

Data collection

Enraf–Nonius MACH3 diffractometer
Absorption correction: none
6093 measured reflections
4298 independent reflections
2704 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
2 standard reflections
frequency: 120 min
intensity decay: 4%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.116
S = 1.00
4298 reflections
239 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H23···N1^{i}	0.858 (19)	2.10 (2)	2.956 (3)	172 (2)

Symmetry code: (i) $-x+1, -y, -z+1$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2220).

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supplementary materials

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2-Anilino-5-benzoyl-4-phenyl-1,3-thiazole

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Comment

Aminothiazoles constitute excellent precursors of a large variety of biologically active compounds such as inihibitors of human breast cancer cell proliferation (Gorczynski *et al.*, 2004) and as inhibitors of protein phosphatases (Wipf *et al.*, 2001). As a part of our ongoing research focused on the use of N-functionalized imidates in heterocyclic syntheses (El Efrit *et al.*, 1996, Dridi *et al.*, 1998), we show that, in presence of sodium hydride (NaH), the reaction of *N*-thiocarbamoylimidate, Ph—C(OMe)=N—C(NHPh)=S, with 2-Bromo-1-phenylethanone (Br—CH2—C(O)—Ph) can can theoretically lead to thiazole or diazole isomeric ring.

From the X-Ray diffraction experiment, the title compound was identified as 5-Benzoyl-2-phenylamino-4-phenylthiazole, $C_{22}H_{16}N_2OS$ (I)·The bond lengths and bond angles observed in this structure exhibit normal values (Allen, 2002). The four rings constituting the molecule (Fig1) named A(C1, C2, C3, N1, S) for the thiazole and B(C5, C6, C7, C8, C9, C10), C(C11, C12, C13, C14, C15, C16) and D(C17, C18, C19, C20, C21, C22) for the phenyl are as expected planar with the largest deviations being 0.016\%A for the thiazole ring, but they are twisted with respect to each other. The dihedral angles between these planes are A^ B= 51,09 (5), A^D = 55,93 (6), AĈ = 49,99 (7), B^ = 45,51 (7), B^D = 33,57 (8) and C^D = 15,82 (13).

The molecules are organized by pairs forming dimer through N—H···N hydrogen bonds building a graph set motif $R^2_2(8)$ (Etter *et al.*, 1990; Bernstein *et al.*, 1995) (Table 1, Fig. 2). The packing is stabilized by van der Waals interactions.

Experimental

To the suspension of sodium hydride (20 mmol) in THF (50 ml) was added drop wise under nitrogen atmosphere with stirring at room temperature a solution of *N*-thiocarbamoylimidate: Ph—C(OMe)=N—C(NHPh)=S (10 mmol) in THF (10 ml). After stirring for 1 h, 2-Bromo-1-phenylethanone (10 mmol) dissolved in THF (30 ml) was added. The reaction mixture was stirred for a period of 14 h and hydrolyzed with water (10 ml). The organic layer was extracted with chloroform, dried over MgSO4 and concentrated under reduced pressure to give the 5-Benzoyl-2-phenylamino-4-phenylthiazole. Recristallization from water-ethanol (2:1) afford crystals (mp 473 K) suitable for *x*-ray diffraction study.

Refinement

Aryl H atoms were positioned geometrically and refined using a riding model, with C—H = 0.96 Å. whereas the H atom of the NH groups was found in difference fourier maps.

Figures

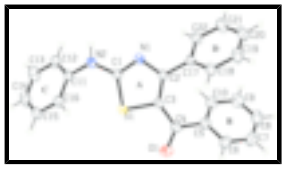

Fig. 1. Molecular view of (I) with the atom-labelling scheme. Ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

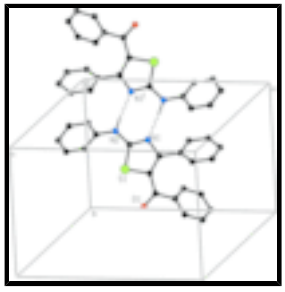

Fig. 2. Partial packing view showing the formation of pseudo dimer through N—H···N hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted for clarity.

2-Anilino-5-benzoyl-4-phenyl-1,3-thiazole

Crystal data

$C_{22}H_{16}N_2OS$	F_{000} = 744
M_r = 356.43	D_x = 1.330 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 25 reflections
a = 13.163 (4) Å	θ = 9–11°
b = 9.433 (4) Å	μ = 0.20 mm^{-1}
c = 14.533 (2) Å	T = 293 (2) K
β = 99.33 (2)°	Prism, colourless
V = 1780.7 (10) Å^3	0.20 × 0.18 × 0.16 mm
Z = 4	

Data collection

Enraf–Nonius MACH3 diffractometer	R_{int} = 0.028
Radiation source: fine-focus sealed tube	θ_{max} = 28.0°
Monochromator: graphite	θ_{min} = 2.3°
T = 293(2) K	h = −17→17
non–profiled ω scans	k = 0→12
Absorption correction: none	l = −5→19
6093 measured reflections	2 standard reflections
4298 independent reflections	every 120 min
2704 reflections with $I > 2\sigma(I)$	intensity decay: 4%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.2524P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.014$
4298 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
239 parameters	$\Delta\rho_{min} = -0.27$ 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 $F^2 > 2$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}
H23	0.4049 (15)	0.014 (2)	0.5334 (15)	0.051 (6)*
S1	0.45331 (4)	0.35859 (5)	0.61163 (4)	0.04442 (15)
N1	0.55404 (11)	0.16658 (16)	0.53728 (11)	0.0406 (4)
N2	0.38926 (12)	0.09407 (19)	0.55532 (13)	0.0474 (4)
C1	0.46481 (13)	0.19246 (19)	0.56396 (13)	0.0393 (4)
C2	0.61980 (13)	0.2793 (2)	0.55837 (13)	0.0393 (4)
C3	0.58128 (13)	0.3926 (2)	0.60089 (14)	0.0419 (5)
C4	0.62158 (16)	0.5284 (2)	0.63774 (14)	0.0485 (5)
C5	0.73535 (16)	0.5524 (2)	0.66124 (14)	0.0473 (5)
C6	0.77439 (18)	0.6847 (2)	0.64381 (15)	0.0582 (6)
H6	0.7307	0.7557	0.6163	0.070*
C7	0.8793 (2)	0.7100 (3)	0.66781 (18)	0.0721 (8)
H7	0.9059	0.7980	0.6553	0.087*
C8	0.9439 (2)	0.6068 (3)	0.70969 (19)	0.0771 (8)
H8	1.0141	0.6246	0.7247	0.093*
C9	0.90544 (18)	0.4770 (3)	0.72957 (17)	0.0698 (7)
H9	0.9491	0.4080	0.7597	0.084*

C10	0.80140 (17)	0.4493 (3)	0.70459 (15)	0.0557 (6)
H10	0.7756	0.3608	0.7170	0.067*
C11	0.30362 (13)	0.0973 (2)	0.60371 (14)	0.0431 (5)
C12	0.28562 (15)	−0.0198 (2)	0.65595 (15)	0.0549 (6)
H12	0.3287	−0.0984	0.6588	0.066*
C13	0.20274 (18)	−0.0194 (3)	0.70408 (17)	0.0692 (7)
H13	0.1900	−0.0985	0.7387	0.083*
C14	0.13943 (16)	0.0965 (3)	0.70108 (17)	0.0674 (7)
H14	0.0850	0.0968	0.7347	0.081*
C15	0.15660 (15)	0.2113 (3)	0.64847 (17)	0.0606 (6)
H15	0.1134	0.2897	0.6461	0.073*
C16	0.23814 (14)	0.2122 (2)	0.59834 (15)	0.0502 (5)
H16	0.2484	0.2898	0.5615	0.060*
C17	0.72450 (13)	0.2650 (2)	0.53328 (13)	0.0408 (4)
C18	0.76104 (16)	0.3639 (2)	0.47657 (16)	0.0547 (5)
H18	0.7196	0.4392	0.4523	0.066*
C19	0.85990 (18)	0.3503 (3)	0.45611 (18)	0.0711 (7)
H19	0.8847	0.4172	0.4183	0.085*
C20	0.92083 (17)	0.2400 (3)	0.49075 (19)	0.0731 (7)
H20	0.9870	0.2318	0.4767	0.088*
C21	0.88460 (16)	0.1402 (3)	0.54673 (18)	0.0671 (7)
H21	0.9266	0.0652	0.5706	0.080*
C22	0.78631 (15)	0.1514 (2)	0.56741 (15)	0.0520 (5)
H22	0.7615	0.0830	0.6042	0.062*
O1	0.56177 (12)	0.62208 (16)	0.65279 (13)	0.0742 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0376 (2)	0.0432 (3)	0.0558 (3)	0.0025 (2)	0.0174 (2)	−0.0052 (3)
N1	0.0362 (8)	0.0400 (9)	0.0481 (10)	−0.0007 (7)	0.0145 (7)	−0.0031 (7)
N2	0.0410 (9)	0.0445 (10)	0.0617 (11)	−0.0052 (7)	0.0230 (8)	−0.0115 (9)
C1	0.0374 (9)	0.0407 (10)	0.0422 (11)	0.0026 (8)	0.0134 (8)	−0.0002 (9)
C2	0.0365 (9)	0.0427 (10)	0.0406 (10)	0.0014 (8)	0.0117 (8)	0.0032 (9)
C3	0.0352 (9)	0.0443 (11)	0.0482 (11)	−0.0001 (8)	0.0127 (8)	−0.0010 (9)
C4	0.0529 (12)	0.0457 (11)	0.0504 (12)	−0.0044 (9)	0.0191 (10)	−0.0063 (10)
C5	0.0546 (12)	0.0509 (12)	0.0397 (11)	−0.0114 (10)	0.0170 (10)	−0.0102 (10)
C6	0.0714 (15)	0.0546 (13)	0.0521 (14)	−0.0146 (11)	0.0207 (12)	−0.0103 (11)
C7	0.0790 (18)	0.0737 (17)	0.0692 (17)	−0.0358 (15)	0.0286 (15)	−0.0197 (14)
C8	0.0570 (14)	0.107 (2)	0.0690 (17)	−0.0226 (15)	0.0163 (13)	−0.0289 (17)
C9	0.0598 (15)	0.0902 (19)	0.0570 (15)	−0.0034 (14)	0.0024 (12)	−0.0135 (14)
C10	0.0585 (13)	0.0642 (14)	0.0458 (12)	−0.0083 (11)	0.0124 (10)	−0.0024 (11)
C11	0.0331 (9)	0.0540 (12)	0.0441 (11)	−0.0052 (8)	0.0118 (8)	−0.0067 (10)
C12	0.0452 (11)	0.0633 (14)	0.0579 (13)	0.0009 (10)	0.0136 (10)	0.0066 (11)
C13	0.0579 (14)	0.0921 (19)	0.0614 (15)	−0.0082 (14)	0.0215 (12)	0.0202 (14)
C14	0.0439 (12)	0.105 (2)	0.0586 (14)	−0.0058 (13)	0.0232 (11)	−0.0032 (15)
C15	0.0382 (11)	0.0757 (16)	0.0706 (16)	0.0028 (11)	0.0165 (11)	−0.0123 (13)
C16	0.0410 (10)	0.0538 (12)	0.0576 (13)	−0.0037 (9)	0.0138 (10)	−0.0061 (11)

C17	0.0335 (9)	0.0454 (11)	0.0452 (11)	−0.0011 (8)	0.0112 (8)	−0.0045 (9)
C18	0.0515 (11)	0.0543 (12)	0.0628 (14)	0.0011 (10)	0.0229 (11)	0.0072 (12)
C19	0.0593 (14)	0.0791 (17)	0.0835 (18)	−0.0054 (13)	0.0375 (13)	0.0095 (15)
C20	0.0392 (11)	0.097 (2)	0.0884 (19)	0.0019 (13)	0.0263 (12)	−0.0029 (17)
C21	0.0428 (11)	0.0779 (16)	0.0802 (17)	0.0152 (12)	0.0090 (12)	0.0066 (15)
C22	0.0427 (10)	0.0573 (13)	0.0570 (13)	0.0026 (10)	0.0111 (10)	0.0042 (11)
O1	0.0654 (10)	0.0550 (10)	0.1070 (14)	0.0013 (8)	0.0286 (10)	−0.0236 (10)

Geometric parameters (Å, °)

S1—C1	1.730 (2)	C11—C16	1.380 (3)
S1—C3	1.7465 (18)	C11—C12	1.382 (3)
N1—C1	1.318 (2)	C12—C13	1.388 (3)
N1—C2	1.374 (2)	C12—H12	0.9300
N2—C1	1.351 (2)	C13—C14	1.371 (3)
N2—C11	1.423 (2)	C13—H13	0.9300
N2—H23	0.86 (2)	C14—C15	1.366 (3)
C2—C3	1.372 (3)	C14—H14	0.9300
C2—C17	1.488 (2)	C15—C16	1.392 (3)
C3—C4	1.456 (3)	C15—H15	0.9300
C4—O1	1.226 (2)	C16—H16	0.9300
C4—C5	1.498 (3)	C17—C18	1.382 (3)
C5—C10	1.386 (3)	C17—C22	1.387 (3)
C5—C6	1.388 (3)	C18—C19	1.387 (3)
C6—C7	1.389 (3)	C18—H18	0.9300
C6—H6	0.9300	C19—C20	1.360 (3)
C7—C8	1.369 (4)	C19—H19	0.9300
C7—H7	0.9300	C20—C21	1.379 (3)
C8—C9	1.374 (4)	C20—H20	0.9300
C8—H8	0.9300	C21—C22	1.379 (3)
C9—C10	1.383 (3)	C21—H21	0.9300
C9—H9	0.9300	C22—H22	0.9300
C10—H10	0.9300		
C1—S1—C3	88.98 (9)	C16—C11—N2	121.77 (19)
C1—N1—C2	110.51 (15)	C12—C11—N2	118.35 (18)
C1—N2—C11	124.74 (17)	C11—C12—C13	119.5 (2)
C1—N2—H23	114.9 (13)	C11—C12—H12	120.2
C11—N2—H23	117.4 (14)	C13—C12—H12	120.2
N1—C1—N2	121.53 (17)	C14—C13—C12	120.6 (2)
N1—C1—S1	115.19 (14)	C14—C13—H13	119.7
N2—C1—S1	123.27 (14)	C12—C13—H13	119.7
C3—C2—N1	115.96 (15)	C15—C14—C13	119.7 (2)
C3—C2—C17	127.27 (17)	C15—C14—H14	120.2
N1—C2—C17	116.77 (16)	C13—C14—H14	120.2
C2—C3—C4	135.42 (17)	C14—C15—C16	120.6 (2)
C2—C3—S1	109.24 (14)	C14—C15—H15	119.7
C4—C3—S1	115.35 (14)	C16—C15—H15	119.7
O1—C4—C3	119.58 (19)	C11—C16—C15	119.6 (2)
O1—C4—C5	119.83 (19)	C11—C16—H16	120.2

C3—C4—C5	120.54 (18)	C15—C16—H16	120.2
C10—C5—C6	119.4 (2)	C18—C17—C22	119.60 (18)
C10—C5—C4	121.85 (19)	C18—C17—C2	120.71 (18)
C6—C5—C4	118.7 (2)	C22—C17—C2	119.69 (17)
C5—C6—C7	119.4 (2)	C17—C18—C19	119.6 (2)
C5—C6—H6	120.3	C17—C18—H18	120.2
C7—C6—H6	120.3	C19—C18—H18	120.2
C8—C7—C6	120.7 (2)	C20—C19—C18	120.6 (2)
C8—C7—H7	119.7	C20—C19—H19	119.7
C6—C7—H7	119.7	C18—C19—H19	119.7
C7—C8—C9	120.2 (2)	C19—C20—C21	120.1 (2)
C7—C8—H8	119.9	C19—C20—H20	120.0
C9—C8—H8	119.9	C21—C20—H20	120.0
C8—C9—C10	119.7 (3)	C20—C21—C22	120.2 (2)
C8—C9—H9	120.1	C20—C21—H21	119.9
C10—C9—H9	120.1	C22—C21—H21	119.9
C9—C10—C5	120.5 (2)	C21—C22—C17	119.9 (2)
C9—C10—H10	119.7	C21—C22—H22	120.1
C5—C10—H10	119.7	C17—C22—H22	120.1
C16—C11—C12	119.87 (18)		
C2—N1—C1—N2	−176.33 (18)	C7—C8—C9—C10	1.9 (4)
C2—N1—C1—S1	2.8 (2)	C8—C9—C10—C5	−1.2 (3)
C11—N2—C1—N1	162.18 (19)	C6—C5—C10—C9	−0.6 (3)
C11—N2—C1—S1	−16.8 (3)	C4—C5—C10—C9	−176.8 (2)
C3—S1—C1—N1	−3.38 (16)	C1—N2—C11—C16	55.9 (3)
C3—S1—C1—N2	175.70 (18)	C1—N2—C11—C12	−125.2 (2)
C1—N1—C2—C3	−0.3 (2)	C16—C11—C12—C13	−1.3 (3)
C1—N1—C2—C17	179.33 (16)	N2—C11—C12—C13	179.8 (2)
N1—C2—C3—C4	177.6 (2)	C11—C12—C13—C14	−0.7 (4)
C17—C2—C3—C4	−2.1 (4)	C12—C13—C14—C15	1.5 (4)
N1—C2—C3—S1	−2.1 (2)	C13—C14—C15—C16	−0.4 (4)
C17—C2—C3—S1	178.25 (16)	C12—C11—C16—C15	2.4 (3)
C1—S1—C3—C2	2.93 (15)	N2—C11—C16—C15	−178.74 (19)
C1—S1—C3—C4	−176.84 (16)	C14—C15—C16—C11	−1.6 (3)
C2—C3—C4—O1	163.3 (2)	C3—C2—C17—C18	−56.6 (3)
S1—C3—C4—O1	−17.0 (3)	N1—C2—C17—C18	123.8 (2)
C2—C3—C4—C5	−19.4 (4)	C3—C2—C17—C22	123.2 (2)
S1—C3—C4—C5	160.29 (15)	N1—C2—C17—C22	−56.4 (3)
O1—C4—C5—C10	136.6 (2)	C22—C17—C18—C19	−1.4 (3)
C3—C4—C5—C10	−40.7 (3)	C2—C17—C18—C19	178.4 (2)
O1—C4—C5—C6	−39.6 (3)	C17—C18—C19—C20	0.5 (4)
C3—C4—C5—C6	143.1 (2)	C18—C19—C20—C21	0.1 (4)
C10—C5—C6—C7	1.7 (3)	C19—C20—C21—C22	0.3 (4)
C4—C5—C6—C7	178.04 (19)	C20—C21—C22—C17	−1.3 (4)
C5—C6—C7—C8	−1.0 (4)	C18—C17—C22—C21	1.8 (3)
C6—C7—C8—C9	−0.8 (4)	C2—C17—C22—C21	−178.0 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H23···N1^{i}	0.858 (19)	2.10 (2)	2.956 (3)	172 (2)

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1.

Fig. 1

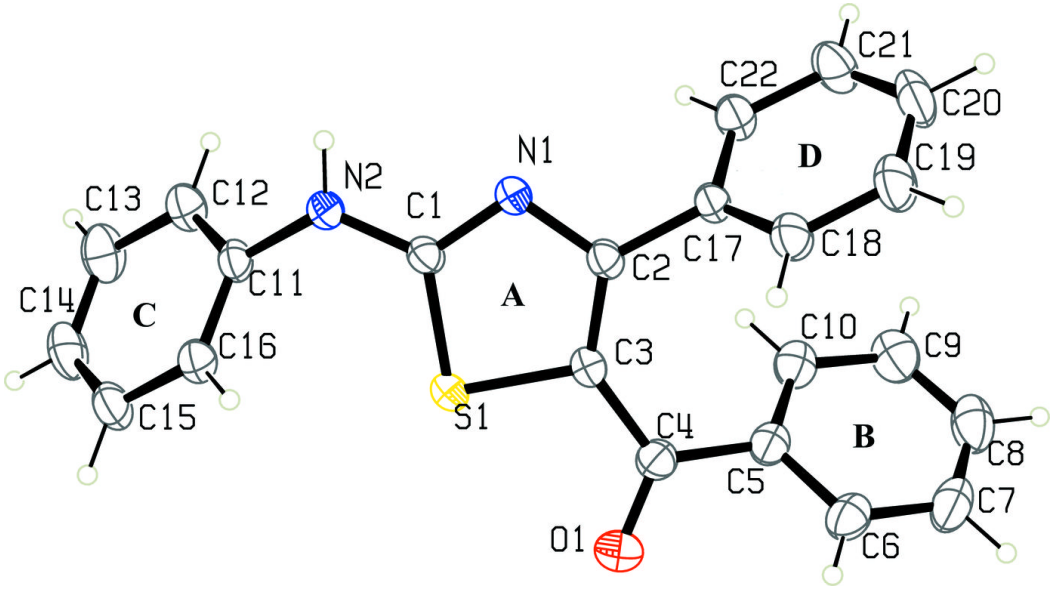
C21
C22
C20
C19
D
N1
N2
C1
C13
C12
C17
C18
C2
C14
C11
A
C
C16
C10
C9
C3
S1
C4
B
C8
C5
C7
O1
C6

Fig. 2