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Ethyl 2-methyl-1-(4-phenylthiazol-2-yl)-1*H*-benzimidazole-6-carboxylate

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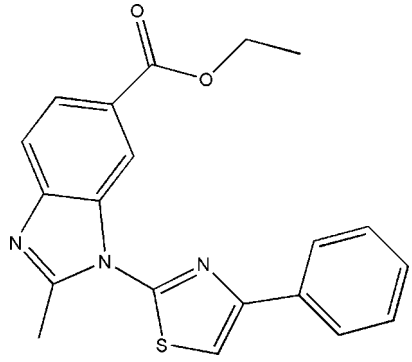
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.107; data-to-parameter ratio = 14.2.

The title compound, $C_{20}H_{17}N_3O_2S$, was prepared by the reaction of ethyl 4-acetamido-3-thioureidobenzoate with 2-bromo-1-phenylethanone in acetone under reflux, followed by neutralization with ammonia. The molecule contains a nonplanar benzimidazole system, displaying a dihedral angle of 1.24 (8)°. The dihedral angle between the thiazole and phenyl rings is 3.62 (5)°. The crystal structure is stabilized by C—H···O hydrogen bonding. The molecules are packed in a face-to-face arrangement showing π–π stacking (centroid-to-centroid distance 3.804 Å).

Related literature

For general background, see: Turan-Zitouni *et al.* (2003).



Experimental

Crystal data

$C_{20}H_{17}N_3O_2S$
M_r = 363.44
Triclinic, $P\overline{1}$
a = 7.4220 (4) Å
b = 10.2999 (6) Å
c = 12.9328 (7) Å
α = 109.850 (1)°
β = 100.866 (1)°
γ = 101.950 (1)°
V = 873.04 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 173 (2) K
0.48 × 0.41 × 0.15 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: none
6843 measured reflections
3373 independent reflections
2789 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.107
S = 1.09
3373 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O1^{i}	0.95	2.35	3.283 (2)	166
C16—H16···O1^{i}	0.95	2.44	3.307 (3)	151

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2301).

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supplementary materials

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Ethyl 2-methyl-1-(4-phenylthiazol-2-yl)-1*H*-benzimidazole-6-carboxylate

L.-M. He, A.-X. Hu, G. Cao and J.-J. Peng

Comment

Heterocyclic compounds containing thiazole ring and benzimidazole rings generally exhibit broad-spectrum biological activity. They were ususlly studied for their antitumor, antiviral and antimicrobial activities (Turan-Zitouni *et al.*, 2003). We report here the synthesis and structure of the title benzimidazole thiazole derivative(I).

The molecular structure of the title compound is illustrated in Fig. 1. The molecule contains four aromatic rings. The large steric effect of the thiazole substituents results in benzyl ring and imidazole ring in the benzimidazole rings being non-coplanar with dihedral angles of 1.24 (8)°. The dihedral angle between the thiazole ring and the least-squares planes of the benzene ring (C15—C20) is 3.62 (5)°. The molecules were associated *via* C—H···O hydrogen bonds (Table 1) and the crystal structure is further stabilized by van der Waals forces. Adjacent benzene units in the benzimidazole rings are exactly parallel and the centroid–centroid distances is 3.804 Å.

Experimental

Ethyl 4-acetamido-3-thioureidobenzoate (5 mmol) and 2-bromo-1-phenyl-ethanone (5 mmol) were dissolved in 50 ml acetone, then the solution was refluxed, the course of the reaction was followed by thin-layer chromatography. After the reaction had finished (about 40 min), the mixture was cooled to room temperature and filtered, the white solid was obtained. The solid product was dissolved in 10 ml e thanol, drop ammonia till pH = 9, a yellow precipitate appeared, which was filtered off and dried to obtain the title compound. Crystals suitable for X-ray crystallographic analysis were obtained by slow evaporation of an ethanol solution at room temperature.

Refinement

Methyl H atoms were placed in calculated positions with C—H = 0.98 Å and torsion angles were refined, with U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were placed in geometrically idealized positions and refined as riding, with C—H = 0.99 (methylene) and 0.95 Å (aromatic), U_{iso}(H)= 1.2U_{eq}(C).

Figures

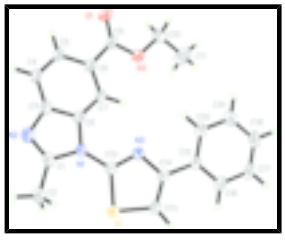

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

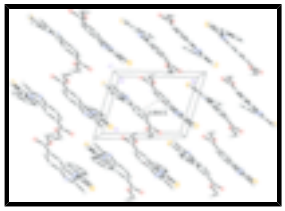

Fig. 2. The crystal packing for (I), showing π-π stacking interactions as dashed lines.

Ethyl 2-methyl-1-(4-phenylthiazol-2-yl)-1*H*-benzimidazole-6-carboxylate

Crystal data

$C_{20}H_{17}N_3O_2S$	$Z = 2$
$M_r = 363.44$	$F_{000} = 380$
Triclinic, $P\overline{1}$	$D_x = 1.383$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.4220$ (4) Å	Cell parameters from 4266 reflections
$b = 10.2999$ (6) Å	$\theta = 2.2$–27.0°
$c = 12.9328$ (7) Å	$\mu = 0.21$ mm^{-1}
$\alpha = 109.850$ (1)°	$T = 173$ (2) K
$\beta = 100.866$ (1)°	Plate, yellow
$\gamma = 101.950$ (1)°	0.48 × 0.41 × 0.15 mm
$V = 873.04$ (8) Å^3	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	2789 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.026$
Monochromator: graphite	$\theta_{max} = 26.0^\circ$
$T = 173(2)$ K	$\theta_{min} = 1.7^\circ$
φ and ω scans	$h = -9\rightarrow9$
Absorption correction: none	$k = -12\rightarrow12$
6843 measured reflections	$l = -15\rightarrow15$
3373 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.107$	$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.3963P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = 0.001$
3373 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
237 parameters	$\Delta\rho_{min} = -0.26$ 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 $F^2 > 2\text{sigma}(F^2)$ 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}
S1	0.15728 (6)	−0.11625 (5)	0.37067 (4)	0.02891 (15)
C1	0.2904 (3)	0.0828 (2)	0.22862 (15)	0.0288 (4)
C2	0.1496 (3)	−0.0595 (2)	0.15201 (16)	0.0381 (5)
H2A	0.1177	−0.0651	0.0732	0.057*
H2B	0.0328	−0.0702	0.1772	0.057*
H2C	0.2053	−0.1369	0.1551	0.057*
C3	0.4919 (3)	0.2931 (2)	0.28858 (15)	0.0287 (4)
C4	0.6071 (3)	0.4251 (2)	0.29823 (16)	0.0323 (4)
H4	0.6029	0.4486	0.2331	0.039*
C5	0.7263 (3)	0.5196 (2)	0.40374 (16)	0.0313 (4)
H5	0.8041	0.6101	0.4117	0.038*
C6	0.7356 (3)	0.48484 (19)	0.50072 (15)	0.0267 (4)
C7	0.6201 (2)	0.35458 (18)	0.49293 (14)	0.0240 (4)
H7	0.6245	0.3309	0.5580	0.029*
C8	0.4988 (2)	0.26145 (18)	0.38600 (14)	0.0243 (4)
C9	0.8658 (3)	0.59264 (19)	0.61240 (16)	0.0288 (4)
C10	0.9946 (3)	0.6407 (2)	0.80855 (17)	0.0385 (5)
H10A	0.9371	0.7189	0.8396	0.046*
H10B	1.1251	0.6844	0.8063	0.046*
C11	1.0032 (4)	0.5554 (3)	0.8808 (2)	0.0744 (9)
H11A	0.8743	0.5180	0.8863	0.112*
H11B	1.0887	0.6173	0.9576	0.112*
H11C	1.0523	0.4746	0.8462	0.112*
C12	0.3068 (2)	0.05844 (18)	0.41850 (14)	0.0228 (4)
C13	0.1779 (2)	−0.09185 (19)	0.51055 (15)	0.0269 (4)
H13	0.1158	−0.1622	0.5346	0.032*
C14	0.2952 (2)	0.04196 (18)	0.58256 (15)	0.0238 (4)
C15	0.3498 (2)	0.10339 (19)	0.70895 (14)	0.0247 (4)
C16	0.3088 (3)	0.0173 (2)	0.76966 (16)	0.0317 (4)
H16	0.2450	−0.0830	0.7296	0.038*
C17	0.3611 (3)	0.0781 (2)	0.88837 (17)	0.0390 (5)

H17	0.3330	0.0187	0.9291	0.047*
C18	0.4534 (3)	0.2235 (3)	0.94804 (17)	0.0441 (5)
H18	0.4868	0.2644	1.0294	0.053*
C19	0.4973 (3)	0.3099 (2)	0.88858 (17)	0.0432 (5)
H19	0.5624	0.4100	0.9293	0.052*
C20	0.4463 (3)	0.2503 (2)	0.77009 (16)	0.0336 (4)
H20	0.4771	0.3099	0.7299	0.040*
N1	0.3646 (2)	0.12445 (15)	0.34639 (12)	0.0245 (3)
N2	0.3621 (2)	0.18000 (17)	0.19236 (13)	0.0320 (4)
N3	0.3666 (2)	0.12749 (15)	0.52841 (12)	0.0241 (3)
O1	0.9530 (2)	0.71445 (14)	0.62906 (12)	0.0380 (3)
O2	0.87693 (19)	0.54106 (14)	0.69478 (11)	0.0336 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0304 (3)	0.0264 (2)	0.0251 (2)	0.00200 (18)	0.00595 (18)	0.00911 (18)
C1	0.0339 (10)	0.0339 (10)	0.0218 (9)	0.0142 (8)	0.0092 (7)	0.0117 (8)
C2	0.0417 (11)	0.0416 (11)	0.0236 (9)	0.0060 (9)	0.0047 (8)	0.0101 (8)
C3	0.0389 (10)	0.0311 (10)	0.0252 (9)	0.0169 (8)	0.0145 (8)	0.0150 (8)
C4	0.0469 (12)	0.0354 (10)	0.0307 (10)	0.0186 (9)	0.0217 (9)	0.0227 (8)
C5	0.0384 (10)	0.0309 (10)	0.0380 (10)	0.0135 (8)	0.0215 (9)	0.0217 (8)
C6	0.0295 (9)	0.0271 (9)	0.0303 (9)	0.0105 (8)	0.0136 (8)	0.0154 (8)
C7	0.0286 (9)	0.0260 (9)	0.0254 (9)	0.0106 (7)	0.0128 (7)	0.0152 (7)
C8	0.0289 (9)	0.0253 (9)	0.0259 (9)	0.0108 (7)	0.0130 (7)	0.0142 (7)
C9	0.0284 (9)	0.0291 (10)	0.0375 (10)	0.0101 (8)	0.0155 (8)	0.0192 (8)
C10	0.0342 (11)	0.0384 (11)	0.0344 (11)	0.0035 (9)	0.0031 (9)	0.0119 (9)
C11	0.081 (2)	0.0746 (19)	0.0469 (15)	−0.0151 (16)	−0.0070 (14)	0.0343 (14)
C12	0.0232 (8)	0.0247 (9)	0.0234 (8)	0.0084 (7)	0.0080 (7)	0.0112 (7)
C13	0.0271 (9)	0.0285 (9)	0.0274 (9)	0.0062 (7)	0.0087 (7)	0.0142 (8)
C14	0.0238 (8)	0.0252 (9)	0.0262 (9)	0.0079 (7)	0.0089 (7)	0.0132 (7)
C15	0.0237 (8)	0.0304 (9)	0.0245 (9)	0.0092 (7)	0.0106 (7)	0.0134 (7)
C16	0.0292 (9)	0.0373 (10)	0.0324 (10)	0.0064 (8)	0.0109 (8)	0.0192 (8)
C17	0.0368 (11)	0.0576 (13)	0.0302 (10)	0.0093 (10)	0.0127 (9)	0.0273 (10)
C18	0.0455 (12)	0.0607 (14)	0.0240 (10)	0.0105 (11)	0.0131 (9)	0.0154 (10)
C19	0.0517 (13)	0.0411 (12)	0.0286 (10)	0.0077 (10)	0.0113 (9)	0.0074 (9)
C20	0.0440 (11)	0.0298 (10)	0.0291 (10)	0.0092 (9)	0.0131 (9)	0.0135 (8)
N1	0.0289 (8)	0.0265 (8)	0.0200 (7)	0.0079 (6)	0.0082 (6)	0.0110 (6)
N2	0.0422 (9)	0.0359 (9)	0.0244 (8)	0.0158 (7)	0.0123 (7)	0.0156 (7)
N3	0.0284 (8)	0.0236 (7)	0.0220 (7)	0.0065 (6)	0.0079 (6)	0.0111 (6)
O1	0.0395 (8)	0.0298 (7)	0.0443 (8)	0.0011 (6)	0.0127 (7)	0.0190 (6)
O2	0.0359 (7)	0.0298 (7)	0.0307 (7)	0.0000 (6)	0.0049 (6)	0.0148 (6)

Geometric parameters (Å, °)

S1—C13	1.7118 (18)	C10—C11	1.486 (3)
S1—C12	1.7348 (17)	C10—H10A	0.9900
C1—N2	1.303 (2)	C10—H10B	0.9900
C1—N1	1.396 (2)	C11—H11A	0.9800

C1—C2	1.487 (3)	C11—H11B	0.9800
C2—H2A	0.9800	C11—H11C	0.9800
C2—H2B	0.9800	C12—N3	1.292 (2)
C2—H2C	0.9800	C12—N1	1.406 (2)
C3—N2	1.390 (2)	C13—C14	1.360 (2)
C3—C4	1.399 (3)	C13—H13	0.9500
C3—C8	1.399 (2)	C14—N3	1.383 (2)
C4—C5	1.371 (3)	C14—C15	1.476 (2)
C4—H4	0.9500	C15—C16	1.395 (2)
C5—C6	1.410 (2)	C15—C20	1.398 (3)
C5—H5	0.9500	C16—C17	1.386 (3)
C6—C7	1.395 (2)	C16—H16	0.9500
C6—C9	1.481 (3)	C17—C18	1.378 (3)
C7—C8	1.384 (2)	C17—H17	0.9500
C7—H7	0.9500	C18—C19	1.389 (3)
C8—N1	1.407 (2)	C18—H18	0.9500
C9—O1	1.211 (2)	C19—C20	1.384 (3)
C9—O2	1.339 (2)	C19—H19	0.9500
C10—O2	1.449 (2)	C20—H20	0.9500
C13—S1—C12	88.61 (8)	C10—C11—H11B	109.5
N2—C1—N1	112.84 (16)	H11A—C11—H11B	109.5
N2—C1—C2	123.53 (16)	C10—C11—H11C	109.5
N1—C1—C2	123.60 (16)	H11A—C11—H11C	109.5
C1—C2—H2A	109.5	H11B—C11—H11C	109.5
C1—C2—H2B	109.5	N3—C12—N1	120.33 (15)
H2A—C2—H2B	109.5	N3—C12—S1	115.25 (13)
C1—C2—H2C	109.5	N1—C12—S1	124.41 (13)
H2A—C2—H2C	109.5	C14—C13—S1	110.76 (13)
H2B—C2—H2C	109.5	C14—C13—H13	124.6
N2—C3—C4	129.56 (16)	S1—C13—H13	124.6
N2—C3—C8	110.72 (16)	C13—C14—N3	114.64 (15)
C4—C3—C8	119.72 (17)	C13—C14—C15	127.17 (16)
C5—C4—C3	118.58 (16)	N3—C14—C15	118.18 (15)
C5—C4—H4	120.7	C16—C15—C20	118.75 (16)
C3—C4—H4	120.7	C16—C15—C14	121.34 (16)
C4—C5—C6	121.16 (17)	C20—C15—C14	119.91 (15)
C4—C5—H5	119.4	C17—C16—C15	120.09 (18)
C6—C5—H5	119.4	C17—C16—H16	120.0
C7—C6—C5	121.03 (17)	C15—C16—H16	120.0
C7—C6—C9	120.57 (16)	C18—C17—C16	120.83 (18)
C5—C6—C9	118.36 (16)	C18—C17—H17	119.6
C8—C7—C6	116.93 (15)	C16—C17—H17	119.6
C8—C7—H7	121.5	C17—C18—C19	119.61 (18)
C6—C7—H7	121.5	C17—C18—H18	120.2
C7—C8—C3	122.56 (16)	C19—C18—H18	120.2
C7—C8—N1	132.74 (15)	C20—C19—C18	120.0 (2)
C3—C8—N1	104.70 (15)	C20—C19—H19	120.0
O1—C9—O2	122.95 (18)	C18—C19—H19	120.0
O1—C9—C6	124.57 (17)	C19—C20—C15	120.68 (18)

O2—C9—C6	112.48 (15)	C19—C20—H20	119.7
O2—C10—C11	106.65 (17)	C15—C20—H20	119.7
O2—C10—H10A	110.4	C1—N1—C12	129.54 (15)
C11—C10—H10A	110.4	C1—N1—C8	106.00 (14)
O2—C10—H10B	110.4	C12—N1—C8	123.98 (14)
C11—C10—H10B	110.4	C1—N2—C3	105.72 (15)
H10A—C10—H10B	108.6	C12—N3—C14	110.72 (15)
C10—C11—H11A	109.5	C9—O2—C10	116.61 (15)
N2—C3—C4—C5	−179.36 (18)	C16—C17—C18—C19	−1.0 (3)
C8—C3—C4—C5	0.7 (3)	C17—C18—C19—C20	0.8 (3)
C3—C4—C5—C6	0.9 (3)	C18—C19—C20—C15	0.3 (3)
C4—C5—C6—C7	−1.6 (3)	C16—C15—C20—C19	−1.1 (3)
C4—C5—C6—C9	−179.29 (16)	C14—C15—C20—C19	179.53 (18)
C5—C6—C7—C8	0.7 (2)	N2—C1—N1—C12	171.17 (16)
C9—C6—C7—C8	178.32 (15)	C2—C1—N1—C12	−10.8 (3)
C6—C7—C8—C3	0.9 (3)	N2—C1—N1—C8	−1.0 (2)
C6—C7—C8—N1	−179.73 (17)	C2—C1—N1—C8	176.99 (17)
N2—C3—C8—C7	178.39 (16)	N3—C12—N1—C1	−165.96 (16)
C4—C3—C8—C7	−1.7 (3)	S1—C12—N1—C1	14.8 (2)
N2—C3—C8—N1	−1.10 (19)	N3—C12—N1—C8	5.0 (2)
C4—C3—C8—N1	178.81 (16)	S1—C12—N1—C8	−174.28 (13)
C7—C6—C9—O1	−170.71 (17)	C7—C8—N1—C1	−178.19 (18)
C5—C6—C9—O1	7.0 (3)	C3—C8—N1—C1	1.23 (18)
C7—C6—C9—O2	9.0 (2)	C7—C8—N1—C12	9.1 (3)
C5—C6—C9—O2	−173.34 (15)	C3—C8—N1—C12	−171.50 (15)
C13—S1—C12—N3	0.32 (14)	N1—C1—N2—C3	0.3 (2)
C13—S1—C12—N1	179.60 (15)	C2—C1—N2—C3	−177.68 (17)
C12—S1—C13—C14	−0.89 (13)	C4—C3—N2—C1	−179.39 (19)
S1—C13—C14—N3	1.30 (19)	C8—C3—N2—C1	0.5 (2)
S1—C13—C14—C15	−179.55 (14)	N1—C12—N3—C14	−178.97 (14)
C13—C14—C15—C16	11.1 (3)	S1—C12—N3—C14	0.34 (19)
N3—C14—C15—C16	−169.78 (16)	C13—C14—N3—C12	−1.1 (2)
C13—C14—C15—C20	−169.58 (18)	C15—C14—N3—C12	179.71 (14)
N3—C14—C15—C20	9.5 (2)	O1—C9—O2—C10	2.3 (3)
C20—C15—C16—C17	0.9 (3)	C6—C9—O2—C10	−177.43 (15)
C14—C15—C16—C17	−179.74 (16)	C11—C10—O2—C9	−173.47 (19)
C15—C16—C17—C18	0.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O1^{i}	0.95	2.35	3.283 (2)	166
C16—H16···O1^{i}	0.95	2.44	3.307 (3)	151

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

Fig. 1

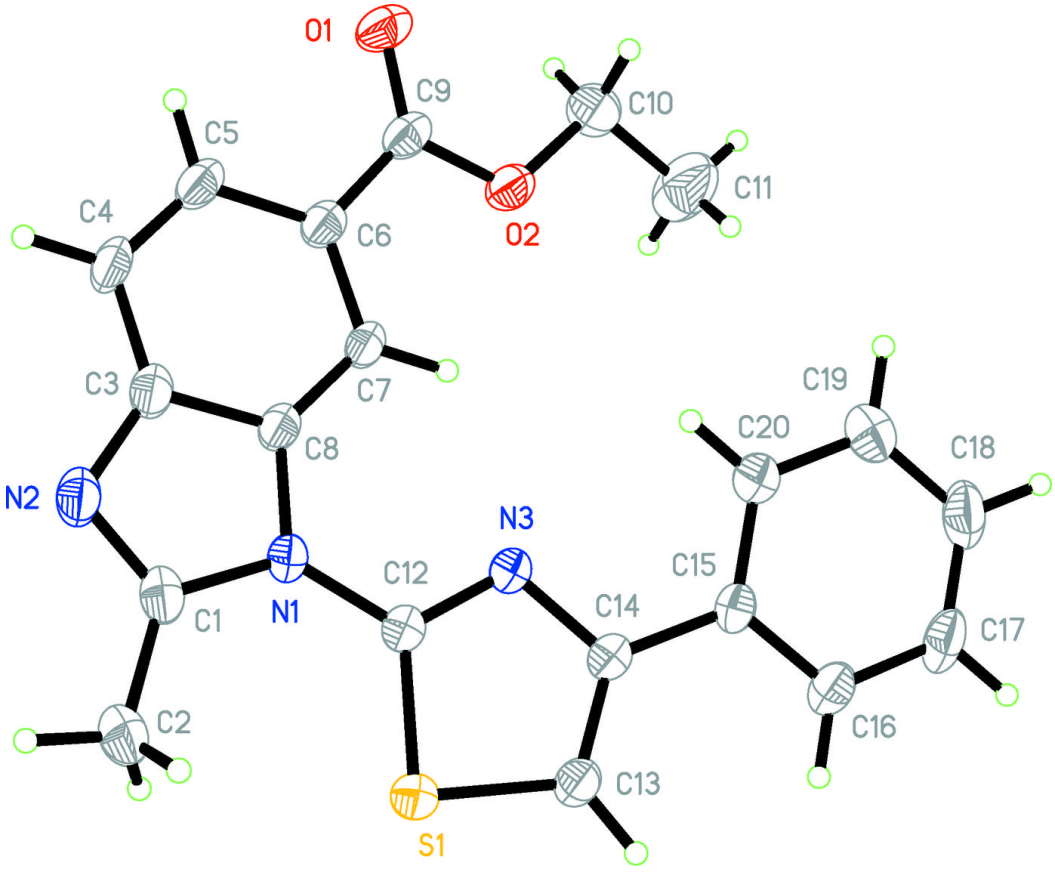
O1
C9
C10
C5
C11
C4
C6
O2
C3
C7
C19
C20
C8
C18
N2
N3
C15
C12
C14
C1
N1
C17
C2
C16
C13
S1

Fig. 2