Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Bromophenyl)-2-(2-thienyl)-acetamide

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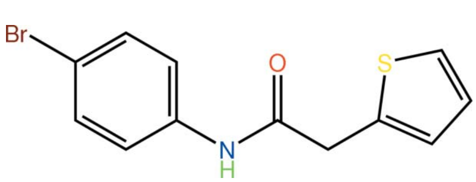
Received 8 December 2009; accepted 11 December 2009

Key indicators: single-crystal X-ray study; *T* = 120 K; mean σ(C–C) = 0.005 Å; disorder in main residue; *R* factor = 0.031; *wR* factor = 0.115; data-to-parameter ratio = 12.7.

The thienyl ring in the title compound, $C_{12}H_{10}BrNOS$, is disordered over two diagonally opposite positions, the major component having a site-occupancy factor of 0.660 (5). The molecule is twisted as evidenced by the dihedral angles of 70.0 (4) and 70.5 (6)° formed between the benzene ring and the two orientations of the disordered thiophene ring. Linear supramolecular chains along the *a* axis are found in the crystal structure through the agency of N—H···O hydrogen bonding.

Related literature

For background to the various applications of 2-substituted thiophenes, see: Campaigne (1984); Kleemann *et al.* (2006). For recent biological studies on 2-substituted thiophenes, see: Lourenço *et al.* (2007). For the structure of the *N*-(2,6-dimethylphenyl) derivative, see: Ferreira *et al.* (2009).



Experimental

Crystal data

$C_{12}H_{10}BrNOS$
M_r = 296.18
Triclinic, $P\bar{1}$
a = 4.7517 (2) Å
b = 10.7283 (3) Å
c = 11.7964 (3) Å
α = 76.419 (2)°
β = 88.437 (2)°
γ = 84.479 (2)°
V = 581.82 (3) Å^3
Z = 2
Mo *Kα* radiation
μ = 3.69 mm^{-1}
T = 120 K
0.09 × 0.06 × 0.02 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.845, T_{max} = 1.000
9757 measured reflections
2045 independent reflections
1847 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.115
S = 0.98
2045 reflections
161 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1n···O1^{i}	0.88 (2)	2.00 (2)	2.848 (3)	162 (3)

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2009).

The use of the EPSRC X-ray crystallographic service at the University of Southampton, England and the valuable assistance of the staff there is gratefully acknowledged. JLW acknowledges support from CAPES (Brazil).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2617).

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supplementary materials

Acta Cryst. (2010). E**66**, o177 [doi:10.1107/S1600536809053355]

N-(4-Bromophenyl)-2-(2-thienyl)acetamide

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Comment

The various uses, for example, as dyestuffs, flavour agents, drugs, and inhibitors, have been well documented for 2-substituted thiophenes related to the title compound (Campaigne, 1984). Thiophenes are present in many natural and synthetic products that have a wide range of pharmacological activities (Kleemann *et al.*, 2006). The *in vitro* antimycobacterial activities of a series of *N*-(aryl)-2-thiophen-2-ylacetamide derivatives were recently investigated and encouraging activities were detected for some of these (Lourenço *et al.*, 2007). The search for new drugs having antibacterial activity against Mycobacterium tuberculosis is a vital task due to the increase of multi-drug resistant tuberculosis (MDR-TB) and AIDS cases worldwide, and the increasing resistance to the currently used main line drugs such as isoniazid and rifampin (http://www.who.int/tdr/diseases/tb/default.htm). Recently, we reported the structure of *N*-(2,6-dimethylphenyl)-2-(thiophen-2-yl)acetamide (Ferreira *et al.*, 2009) and as a continuation of these studies, the title thiophene derivative, (I), is described.

The molecular structure of (I), Fig. 1, is twisted as seen in the values of the C6–N1–C7–C8 and S1–C1–C5–C6 torsion angles of 35.0 (5) and 88.4 (4) °, respectively; the S1'–C1–C5–C6 torsion angle for the minor component of the disordered thiophene ring is -89.9 (5) °. The dihedral angle formed between the thiophene and benzene rings is 70.0 (4) °; the equivalent angle involving the minor component of the thiophene ring is 70.5 (6) °. The anti-conformation of the amide group allows for the formation of linear supramolecular chains along the *a* axis *via* N–H···O hydrogen bonding, Fig. 2 and Table 1.

Experimental

A solution of 4-bromoaniline (2 mmol) and 2-thienylacetyl chloride (2 mmol) in tetrahydrofuran (20 ml) was stirred for 2 h at room temperature, water (30 ml) added and the mixture was extracted with ethyl acetate (2 *x* 20 ml). The combined organic layers were washed with saturated aqueous $NaHCO_3$ and brine, dried over $MgSO_4$, filtered, and rotary evaporated to give the crude product, (yield 96%), which was recrystallized from EtOH; m.pt.: 411–412 K. CG/MS: m/*z* $[M]^{+\cdot}$: 297. ^{1}H NMR [500.00 MHz, DMSO-d_6] δ: 10.30 (1*H*, s, NH), 7.6 (d, 2H, J = 9.0 Hz), 7.48 (d, 2H, J = 9.0 Hz), 7.38, (dd, 1H, J = 4.5 and 2.0 Hz), 6.98–6.96 (m, 2H), 3.87 (s, 2H, CH_2CO) p.p.m.. ^{13}C NMR (125.0 MHz, DMSO-d_6) δ: 168.1, 138.3, 136.8, 131.5, 126.6, 126.3, 125.0, 121.3, 114.8, 37.4 p.p.m.. IR (KBr, cm^{-1}) ν: 1660 (CO).

Refinement

The C-bound H atoms were geometrically placed (C–H = 0.95–0.99 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The N–H atom was located in a difference map and refined with the distance restraint N–H = 0.88±0.01 and with U_{iso}(H) = 1.2U_{eq}(N). The thienyl ring was disordered with two diagonally opposed positions resolved for the S1 and C4 atoms (the anisotropic displacement parameters for the two components of the C4 atom were constrained to be equal). The major component had a site occupancy factor = 0.660 (5).

Figures

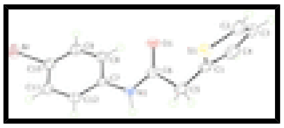
Fig. 1. Molecular structure (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level. Only the major component of the disordered thienyl ring is shown for reasons of clarity.

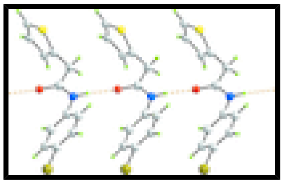
Fig. 2. Supramolecular chain in (I) aligned along the *a* axis and mediated by N–H···O hydrogen bonds (blue dashed lines). Colour code: Br, olive; S, yellow; O, red; N, blue; C, grey; and H, green.

N-(4-Bromophenyl)-2-(2-thienyl)acetamide

Crystal data

$C_{12}H_{10}BrNOS$	$Z = 2$
$M_r = 296.18$	$F(000) = 296$
Triclinic, $P\overline{1}$	$D_x = 1.691$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 4.7517$ (2) Å	Cell parameters from 2592 reflections
$b = 10.7283$ (3) Å	$\theta = 2.9$–$27.5°$
$c = 11.7964$ (3) Å	$\mu = 3.69$ mm^{-1}
$\alpha = 76.419$ (2)°	$T = 120$ K
$\beta = 88.437$ (2)°	Block, pale-brown
$\gamma = 84.479$ (2)°	0.09 × 0.06 × 0.02 mm
$V = 581.82$ (3) Å^3	

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer	2045 independent reflections
Radiation source: Enraf Nonius FR591 rotating anode	1847 reflections with $I > 2\sigma(I)$
10 cm confocal mirrors	$R_{int} = 0.042$
Detector resolution: 9.091 pixels mm^{-1}	$\theta_{max} = 25.0°$, $\theta_{min} = 2.9°$
φ and ω scans	$h = -5 \rightarrow 5$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$k = -12 \rightarrow 12$
$T_{min} = 0.845$, $T_{max} = 1.000$	$l = -14 \rightarrow 14$
9757 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.031$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.115$	H atoms treated by a mixture of independent and constrained refinement
$S = 0.98$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
2045 reflections	$(\Delta/\sigma)_{max} = 0.001$
161 parameters	$\Delta\rho_{max} = 0.40$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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}	Occ. (<1)
Br	0.27885 (7)	−0.23040 (3)	0.97460 (3)	0.03386 (19)	
O1	0.0821 (5)	0.2338 (2)	0.4702 (2)	0.0338 (6)	
N1	0.5204 (5)	0.1924 (3)	0.5506 (2)	0.0237 (6)	
H1N	0.696 (3)	0.211 (3)	0.540 (3)	0.028*	
S1	0.0537 (8)	0.5801 (3)	0.3373 (3)	0.0278 (6)	0.660 (5)
C1	0.2232 (6)	0.4487 (3)	0.3020 (3)	0.0249 (7)	0.660 (5)
C2	−0.1461 (8)	0.6162 (4)	0.2202 (3)	0.0361 (8)	0.660 (5)
H2	−0.2806	0.6894	0.2040	0.043*	0.660 (5)
C3	−0.1056 (7)	0.5346 (4)	0.1488 (3)	0.0318 (8)	0.660 (5)
H3	−0.2006	0.5420	0.0774	0.038*	0.660 (5)
C4	0.108 (4)	0.4342 (19)	0.2003 (15)	0.035 (4)	0.660 (5)
H4	0.1644	0.3633	0.1668	0.042*	0.660 (5)
S1'	0.1360 (17)	0.4123 (9)	0.1850 (6)	0.0245 (14)	0.340 (5)
C1'	0.2232 (6)	0.4487 (3)	0.3020 (3)	0.0249 (7)	0.340 (5)
C2'	−0.1461 (8)	0.6162 (4)	0.2202 (3)	0.0361 (8)	0.340 (5)
H2'	−0.2772	0.6904	0.2108	0.043*	0.340 (5)
C3'	−0.1056 (7)	0.5346 (4)	0.1488 (3)	0.0318 (8)	0.340 (5)
H3'	−0.2134	0.5474	0.0797	0.038*	0.340 (5)
C4'	0.072 (7)	0.561 (3)	0.323 (3)	0.035 (4)	0.340 (5)
H4'	0.0977	0.5980	0.3879	0.042*	0.340 (5)
C5	0.4454 (7)	0.3645 (4)	0.3784 (3)	0.0351 (8)	
H5A	0.5485	0.4183	0.4176	0.042*	
H5B	0.5828	0.3256	0.3290	0.042*	

C6	0.3296 (6)	0.2578 (3)	0.4702 (3)	0.0251 (7)
C7	0.4675 (6)	0.0909 (3)	0.6462 (3)	0.0227 (7)
C8	0.2767 (7)	0.0013 (3)	0.6398 (3)	0.0251 (7)
H8	0.1806	0.0071	0.5689	0.030*
C9	0.2278 (7)	−0.0953 (3)	0.7360 (3)	0.0266 (7)
H9	0.0995	−0.1566	0.7315	0.032*
C10	0.3667 (7)	−0.1026 (3)	0.8397 (3)	0.0252 (7)
C11	0.5612 (7)	−0.0172 (3)	0.8476 (3)	0.0279 (7)
H11	0.6607	−0.0254	0.9181	0.033*
C12	0.6090 (7)	0.0808 (3)	0.7505 (3)	0.0255 (7)
H12	0.7389	0.1414	0.7553	0.031*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0441 (3)	0.0281 (3)	0.0269 (3)	−0.00963 (17)	0.00026 (16)	0.00104 (16)
O1	0.0170 (11)	0.0346 (14)	0.0425 (15)	−0.0075 (10)	−0.0019 (10)	0.0076 (11)
N1	0.0165 (12)	0.0273 (15)	0.0256 (13)	−0.0067 (11)	0.0018 (11)	−0.0008 (11)
S1	0.0324 (10)	0.0221 (11)	0.0298 (12)	−0.0051 (8)	0.0006 (8)	−0.0068 (9)
C1	0.0191 (15)	0.0207 (17)	0.0320 (18)	−0.0039 (12)	0.0043 (13)	−0.0002 (13)
C2	0.0328 (18)	0.0267 (19)	0.042 (2)	−0.0012 (15)	0.0071 (15)	0.0040 (15)
C3	0.0289 (17)	0.039 (2)	0.0236 (17)	−0.0084 (15)	−0.0003 (13)	0.0034 (15)
C4	0.037 (5)	0.038 (7)	0.036 (6)	−0.007 (4)	0.015 (3)	−0.022 (4)
S1'	0.027 (2)	0.029 (3)	0.019 (2)	−0.0057 (17)	0.0037 (17)	−0.007 (2)
C1'	0.0191 (15)	0.0207 (17)	0.0320 (18)	−0.0039 (12)	0.0043 (13)	−0.0002 (13)
C2'	0.0328 (18)	0.0267 (19)	0.042 (2)	−0.0012 (15)	0.0071 (15)	0.0040 (15)
C3'	0.0289 (17)	0.039 (2)	0.0236 (17)	−0.0084 (15)	−0.0003 (13)	0.0034 (15)
C4'	0.037 (5)	0.038 (7)	0.036 (6)	−0.007 (4)	0.015 (3)	−0.022 (4)
C5	0.0228 (16)	0.034 (2)	0.041 (2)	−0.0067 (14)	0.0030 (14)	0.0078 (16)
C6	0.0191 (15)	0.0229 (18)	0.0329 (19)	−0.0039 (13)	0.0040 (13)	−0.0053 (15)
C7	0.0141 (13)	0.0267 (17)	0.0264 (16)	−0.0020 (12)	0.0051 (12)	−0.0050 (13)
C8	0.0278 (16)	0.0224 (17)	0.0257 (16)	−0.0059 (13)	−0.0032 (13)	−0.0048 (13)
C9	0.0254 (16)	0.0235 (17)	0.0317 (17)	−0.0058 (13)	0.0017 (13)	−0.0070 (14)
C10	0.0265 (16)	0.0225 (17)	0.0245 (16)	−0.0022 (13)	0.0025 (13)	−0.0017 (13)
C11	0.0263 (16)	0.0309 (19)	0.0274 (17)	−0.0025 (14)	−0.0008 (13)	−0.0086 (14)
C12	0.0185 (14)	0.0278 (18)	0.0318 (17)	−0.0061 (12)	0.0001 (12)	−0.0087 (14)

Geometric parameters (Å, °)

Br—C10	1.907 (3)	C2'—C3'	1.348 (5)
O1—C6	1.228 (4)	C2'—C4'	1.59 (3)
N1—C6	1.352 (4)	C2'—H2'	0.9500
N1—C7	1.407 (4)	C3'—H3'	0.9500
N1—H1N	0.875 (10)	C4'—H4'	0.9500
S1—C2	1.647 (5)	C5—C6	1.514 (5)
S1—C1	1.687 (4)	C5—H5A	0.9900
C1—C4	1.381 (17)	C5—H5B	0.9900
C1—C5	1.493 (5)	C7—C12	1.396 (4)
C2—C3	1.348 (5)	C7—C8	1.399 (4)

C2—H2	0.9500	C8—C9	1.377 (5)
C3—C4	1.439 (19)	C8—H8	0.9500
C3—H3	0.9500	C9—C10	1.388 (5)
C4—H4	0.9500	C9—H9	0.9500
S1'—C1'	1.594 (8)	C10—C11	1.382 (5)
S1'—C3'	1.641 (9)	C11—C12	1.391 (5)
C1'—C4'	1.42 (3)	C11—H11	0.9500
C1'—C5	1.493 (5)	C12—H12	0.9500

C6—N1—C7	126.1 (3)	C1—C5—C6	113.6 (3)
C6—N1—H1n	117 (2)	C1'—C5—H5A	108.8
C7—N1—H1n	117 (2)	C1—C5—H5A	108.8
C2—S1—C1	93.6 (2)	C6—C5—H5A	108.8
C4—C1—C5	129.6 (8)	C1'—C5—H5B	108.8
C4—C1—S1	108.3 (8)	C1—C5—H5B	108.8
C5—C1—S1	122.0 (3)	C6—C5—H5B	108.8
C3—C2—S1	115.4 (3)	H5A—C5—H5B	107.7
C3—C2—H2	122.3	O1—C6—N1	123.6 (3)
S1—C2—H2	122.3	O1—C6—C5	122.0 (3)
C2—C3—C4	107.7 (7)	N1—C6—C5	114.5 (3)
C2—C3—H3	126.2	C12—C7—C8	119.5 (3)
C4—C3—H3	126.2	C12—C7—N1	118.5 (3)
C1—C4—C3	114.9 (11)	C8—C7—N1	122.1 (3)
C1—C4—H4	122.6	C9—C8—C7	120.1 (3)
C3—C4—H4	122.6	C9—C8—H8	119.9
C1'—S1'—C3'	94.5 (5)	C7—C8—H8	119.9
C4'—C1'—C5	126.1 (14)	C10—C9—C8	119.7 (3)
C4'—C1'—S1'	114.4 (14)	C10—C9—H9	120.2
C5—C1'—S1'	119.4 (4)	C8—C9—H9	120.2
C3'—C2'—C4'	105.2 (11)	C11—C10—C9	121.3 (3)
C3'—C2'—H2'	127.4	C11—C10—Br	119.6 (2)
C4'—C2'—H2'	127.4	C9—C10—Br	119.1 (2)
C2'—C3'—S1'	117.9 (4)	C10—C11—C12	118.9 (3)
C2'—C3'—H3'	121.1	C10—C11—H11	120.5
S1'—C3'—H3'	121.1	C12—C11—H11	120.5
C1'—C4'—C2'	108.0 (19)	C7—C12—C11	120.4 (3)
C1'—C4'—H4'	126.0	C7—C12—H12	119.8
C2'—C4'—H4'	126.0	C11—C12—H12	119.8
C1'—C5—C6	113.6 (3)		

C2—S1—C1—C4	−2.5 (10)	C7—N1—C6—O1	−1.5 (5)
C2—S1—C1—C5	−179.0 (3)	C7—N1—C6—C5	178.7 (3)
C1—S1—C2—C3	0.8 (4)	C1'—C5—C6—O1	9.4 (5)
S1—C2—C3—C4	1.0 (9)	C1—C5—C6—O1	9.4 (5)
C5—C1—C4—C3	179.8 (7)	C1'—C5—C6—N1	−170.8 (3)
S1—C1—C4—C3	3.6 (17)	C1—C5—C6—N1	−170.8 (3)
C2—C3—C4—C1	−3.0 (16)	C6—N1—C7—C12	−144.4 (3)
C3'—S1'—C1'—C4'	−0.6 (19)	C6—N1—C7—C8	35.0 (5)
C3'—S1'—C1'—C5	178.7 (3)	C12—C7—C8—C9	0.5 (5)
C4'—C2'—C3'—S1'	0.1 (13)	N1—C7—C8—C9	−178.9 (3)

C1'—S1'—C3'—C2'	0.3 (6)	C7—C8—C9—C10	0.6 (5)
C5—C1'—C4'—C2'	−178.6 (8)	C8—C9—C10—C11	−2.2 (5)
S1'—C1'—C4'—C2'	1(3)	C8—C9—C10—Br	176.1 (2)
C3'—C2'—C4'—C1'	0(2)	C9—C10—C11—C12	2.6 (5)
C4'—C1'—C5—C6	89.3 (18)	Br—C10—C11—C12	−175.7 (2)
S1'—C1'—C5—C6	−89.9 (5)	C8—C7—C12—C11	0.0 (5)
C4—C1—C5—C6	−87.3 (12)	N1—C7—C12—C11	179.4 (3)
S1—C1—C5—C6	88.4 (4)	C10—C11—C12—C7	−1.5 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1n···O1^{i}	0.875 (17)	2.00 (2)	2.848 (3)	162 (3)

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

Fig. 1

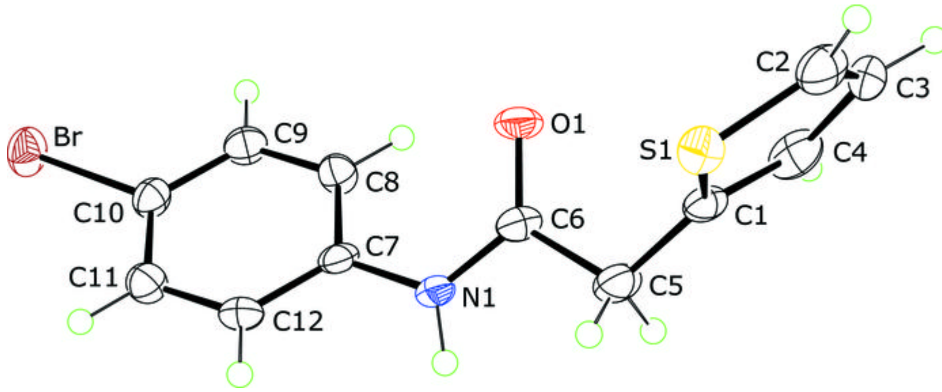

Fig. 2