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(*Z*)-3-(4-Methylphenyl)-2-(3-thienyl)acrylonitrile

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.035
wR factor = 0.096
Data-to-parameter ratio = 18.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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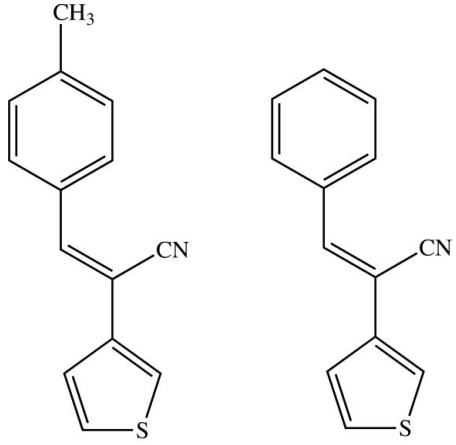
In the molecule of the title compound, $C_{14}H_{11}NS$, the benzene ring is significantly rotated out of the plane of the rest of the molecule. There are no significant direction-specific interactions between the molecules.

Comment

We have recently reported the structures of a number of 3-aryl-2-thienylacrylonitrile derivatives (Cobo *et al.*, 2005, 2006). We report here the structure of the title compound, (I) (Fig. 1), which we compare with that of the phenyl analogue, (II) (Cobo *et al.*, 2006). The molecule of compound (I) is approximately planar apart from the benzene ring, which is significantly rotated out of the plane of the rest of the molecule about the bond C17—C11 (Table 1). The nitrile fragment shows the usual long C—C bond and very short C—N bond, but the rest of the geometry shows no unexpected features. By contrast, the whole molecule of compound (II) is virtually planar, with a C37—C17—C11—C12 torsion angle of only −1.7 (5)°.



(I) (II)

In compound (II), the molecules are linked into sheets by a combination of C—H···N and C—H···π(arene) hydrogen bonds; by contrast, in (I), the shortest non-bonded intermolecular contacts between potential hydrogen-bond donors and acceptors (Table 2) are all too long to be structurally significant, although they involve precisely the same combinations of donors and acceptors as the hydrogen bonds in compound (II). Hence, the introduction of the 4-methyl substituent in compound (I) in place of the 4-H in compound (II) appears to stretch the crystal structure sufficiently to put the corresponding combinations of hydrogen-bond donors and acceptors just out of bonding range.

Experimental

A solution of 3-thiopheneacetonitrile (1 mmol) and potassium *tert*-butoxide (1 mmol) in anhydrous ethanol (3 ml) was stirred at room temperature for 15 min; a solution of 4-methylbenzaldehyde (1 mmol) in anhydrous ethanol (3 ml) was then added and the mixture was set aside until formation of a precipitate was complete. The resulting solid product was collected by filtration, washed with ethanol, dried and finally recrystallized from dimethylformamide to give colourless crystals of (I) suitable for single-crystal X-ray diffraction (yield 60%; m.p. 365–367 K).

Crystal data

$C_{14}H_{11}NS$	$Z = 4$
$M_r = 225.30$	$D_x = 1.304$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 13.7415$ (3) Å	$\mu = 0.25$ mm^{-1}
$b = 10.8492$ (3) Å	$T = 120$ (2) K
$c = 8.0238$ (2) Å	Block, colourless
$\beta = 106.439$ (2)°	0.50 × 0.25 × 0.25 mm
$V = 1147.32$ (5) Å^3	

Data collection

Bruker–Nonius KappaCCD diffractometer	15435 measured reflections
	2628 independent reflections
φ and ω scans	2284 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$R_{int} = 0.027$
	$\theta_{max} = 27.5°$
$T_{min} = 0.885$, $T_{max} = 0.940$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.5552P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.035$	
$wR(F^2) = 0.096$	
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
2628 reflections	$\Delta\rho_{max} = 0.30$ e Å^{-3}
146 parameters	$\Delta\rho_{min} = -0.35$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C37—C371	1.4444 (18)	C371—N37	1.1499 (18)
C2—C3—C37—C17	176.17 (13)	C37—C17—C11—C12	−26.9 (2)
C3—C37—C17—C11	−177.98 (12)		

Table 2
Parameters (Å, °) for short intermolecular contacts.

Cg is the centroid of the C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N37^{i}	0.95	2.75	3.312 (2)	119
C13—H13···*Cg*^{ii}	0.95	2.99	3.777 (2)	141

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

All H atoms were treated as riding atoms, with C—H = 0.98 (CH_3) or 0.95 Å (all other H atoms) and $U_{iso}(H) = kU_{eq}(C)$, where $k = 1.5$ for methyl H atoms and 1.2 for all other H atoms.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

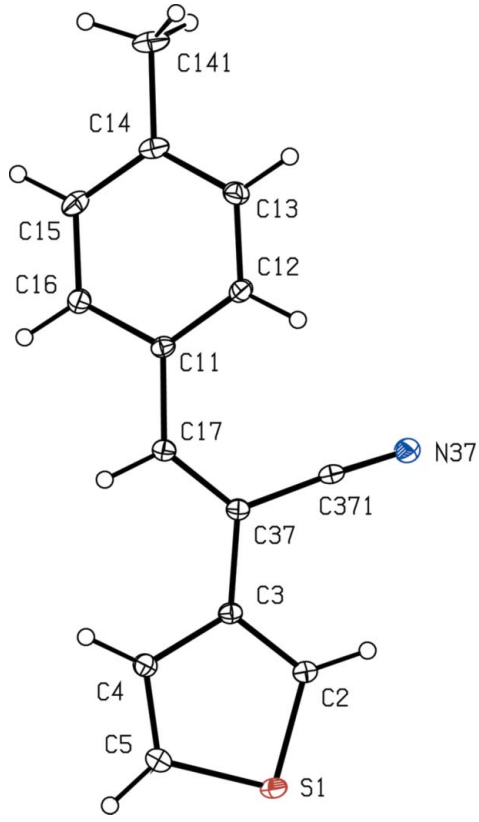


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

X-ray data were collected at the EPSRC National X-ray Crystallography Service, University of Southampton, England. JC and JT thank the Consejería de Innovación, Ciencia y Empresa (Junta de Andalucía, Spain) and the Universidad de Jaén for financial support. DC thanks COLCIENCIAS and UNIVALLE (Universidad del Valle, Colombia) for financial support.

References

Cobo, D., Quiroga, J., Cobo, J., Low, J. N. & Glidewell, C. (2005). *Acta Cryst.* E**61**, o3639–o3641.
Cobo, D., Quiroga, J., de la Torre, J. M., Cobo, J., Low, J. N. & Glidewell, C. (2006). *Acta Cryst.* C**62**, o550–o553.
Ferguson, G. (1999). *PRPKAPPA*. University of Guelph, Canada.
Hooft, R. W. W. (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
McArdle, P. (2003). *OSCAIL for Windows*. Version 10. Crystallography Centre, Chemistry Department, NUI Galway, Ireland.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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$c = 8.0238\ (2)$ Å
$\beta = 106.439\ (2)°$
$V = 1147.32\ (5)$ Å^3
$Z = 4$
$F(000) = 472$
$D_x = 1.304$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2628 reflections
$\theta = 2.4$–$27.5°$
$\mu = 0.25$ mm^{-1}
$T = 120$ K
Block, colourless
0.50 × 0.25 × 0.25 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: Bruker-Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.885$, $T_{max} = 0.940$
15435 measured reflections
2628 independent reflections
2284 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
$h = -17\rightarrow17$
$k = -14\rightarrow14$
$l = -10\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.096$
$S = 1.05$
2628 reflections
146 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.5552P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.33892 (2)	0.22914 (3)	0.23475 (4)	0.02236 (12)
C2	0.45498 (10)	0.19264 (13)	0.37130 (17)	0.0193 (3)
C3	0.51901 (10)	0.29212 (12)	0.40812 (16)	0.0164 (3)

C4	0.47088 (10)	0.40121 (13)	0.32193 (17)	0.0198 (3)
C5	0.37394 (11)	0.37998 (13)	0.22405 (18)	0.0222 (3)
C37	0.62421 (10)	0.28555 (12)	0.52110 (16)	0.0164 (3)
C371	0.65503 (9)	0.16439 (12)	0.59084 (17)	0.0177 (3)
N37	0.67540 (9)	0.06549 (11)	0.63993 (16)	0.0241 (3)
C17	0.69020 (10)	0.38086 (12)	0.55123 (16)	0.0174 (3)
C11	0.79651 (10)	0.38364 (12)	0.65604 (16)	0.0167 (3)
C12	0.83749 (10)	0.30514 (13)	0.79697 (18)	0.0208 (3)
C13	0.93993 (11)	0.30936 (14)	0.88594 (18)	0.0229 (3)
C14	1.00530 (10)	0.39136 (14)	0.83822 (18)	0.0214 (3)
C141	1.11724 (11)	0.39195 (16)	0.9328 (2)	0.0313 (4)
C15	0.96409 (11)	0.47273 (14)	0.70231 (18)	0.0236 (3)
C16	0.86167 (11)	0.46975 (13)	0.61301 (18)	0.0215 (3)
H2	0.4732	0.1124	0.4167	0.023*
H4	0.5030	0.4795	0.3320	0.024*
H5	0.3308	0.4415	0.1576	0.027*
H17	0.6641	0.4565	0.4970	0.021*
H12	0.7946	0.2482	0.8321	0.025*
H13	0.9660	0.2553	0.9813	0.028*
H14A	1.1264	0.3939	1.0584	0.047*
H14B	1.1490	0.4649	0.8985	0.047*
H14C	1.1489	0.3174	0.9029	0.047*
H15	1.0069	0.5313	0.6702	0.028*
H16	0.8353	0.5268	0.5215	0.026*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01510 (19)	0.0265 (2)	0.02236 (19)	−0.00323 (12)	0.00024 (14)	0.00062 (13)
C2	0.0159 (6)	0.0206 (7)	0.0203 (6)	−0.0009 (5)	0.0032 (5)	−0.0001 (5)
C3	0.0145 (6)	0.0196 (7)	0.0155 (6)	0.0000 (5)	0.0049 (5)	−0.0010 (5)
C4	0.0190 (6)	0.0191 (7)	0.0201 (6)	0.0007 (5)	0.0036 (5)	0.0003 (5)
C5	0.0202 (7)	0.0236 (7)	0.0213 (6)	0.0029 (5)	0.0031 (5)	0.0021 (5)
C37	0.0153 (6)	0.0182 (6)	0.0156 (6)	0.0006 (5)	0.0044 (5)	−0.0009 (5)
C371	0.0126 (6)	0.0215 (7)	0.0178 (6)	−0.0021 (5)	0.0020 (5)	−0.0032 (5)
N37	0.0217 (6)	0.0206 (6)	0.0273 (6)	−0.0012 (5)	0.0025 (5)	−0.0012 (5)
C17	0.0164 (6)	0.0188 (6)	0.0164 (6)	0.0005 (5)	0.0035 (5)	−0.0007 (5)
C11	0.0155 (6)	0.0177 (6)	0.0168 (6)	−0.0009 (5)	0.0040 (5)	−0.0033 (5)
C12	0.0194 (7)	0.0214 (7)	0.0202 (6)	−0.0053 (5)	0.0035 (5)	0.0007 (5)
C13	0.0216 (7)	0.0221 (7)	0.0208 (6)	0.0001 (5)	−0.0010 (5)	0.0000 (5)
C14	0.0144 (6)	0.0258 (7)	0.0231 (7)	−0.0010 (5)	0.0035 (5)	−0.0080 (5)
C141	0.0142 (7)	0.0421 (9)	0.0345 (8)	−0.0011 (6)	0.0021 (6)	−0.0088 (7)
C15	0.0202 (7)	0.0274 (8)	0.0243 (7)	−0.0080 (5)	0.0082 (6)	−0.0029 (6)
C16	0.0223 (7)	0.0209 (7)	0.0201 (6)	−0.0031 (5)	0.0040 (5)	0.0015 (5)

Geometric parameters (Å, º)

S1—C2	1.7064 (13)	C11—C12	1.4002 (19)
S1—C5	1.7147 (15)	C11—C16	1.4031 (19)
C2—C3	1.3709 (19)	C12—C13	1.3873 (19)
C2—H2	0.95	C12—H12	0.95
C3—C4	1.4345 (18)	C13—C14	1.393 (2)
C3—C37	1.4748 (17)	C13—H13	0.95
C4—C5	1.3609 (19)	C14—C15	1.393 (2)
C4—H4	0.95	C14—C141	1.5104 (18)
C5—H5	0.95	C141—H14A	0.98
C37—C17	1.3512 (18)	C141—H14B	0.98
C37—C371	1.4444 (18)	C141—H14C	0.98
C371—N37	1.1499 (18)	C15—C16	1.3873 (19)
C17—C11	1.4653 (18)	C15—H15	0.95
C17—H17	0.95	C16—H16	0.95
C2—S1—C5	91.67 (7)	C16—C11—C17	118.33 (12)
C3—C2—S1	112.45 (10)	C13—C12—C11	120.87 (13)
C3—C2—H2	123.8	C13—C12—H12	119.6
S1—C2—H2	123.8	C11—C12—H12	119.6
C2—C3—C4	111.43 (12)	C12—C13—C14	121.27 (13)
C2—C3—C37	123.51 (12)	C12—C13—H13	119.4
C4—C3—C37	125.05 (12)	C14—C13—H13	119.4
C5—C4—C3	112.40 (12)	C15—C14—C13	117.99 (13)
C5—C4—H4	123.8	C15—C14—C141	121.43 (13)
C3—C4—H4	123.8	C13—C14—C141	120.59 (13)
C4—C5—S1	112.05 (11)	C14—C141—H14A	109.5
C4—C5—H5	124.0	C14—C141—H14B	109.5
S1—C5—H5	124.0	H14A—C141—H14B	109.5
C17—C37—C371	121.25 (12)	C14—C141—H14C	109.5
C17—C37—C3	124.36 (12)	H14A—C141—H14C	109.5
C371—C37—C3	114.27 (11)	H14B—C141—H14C	109.5
N37—C371—C37	176.48 (14)	C16—C15—C14	121.19 (13)
C37—C17—C11	128.90 (12)	C16—C15—H15	119.4
C37—C17—H17	115.5	C14—C15—H15	119.4
C11—C17—H17	115.5	C15—C16—C11	120.88 (13)
C12—C11—C16	117.70 (12)	C15—C16—H16	119.6
C12—C11—C17	123.97 (12)	C11—C16—H16	119.6
C5—S1—C2—C3	−0.05 (11)	C37—C17—C11—C12	−26.9 (2)
S1—C2—C3—C4	0.22 (15)	C37—C17—C11—C16	152.97 (14)
S1—C2—C3—C37	−179.23 (10)	C16—C11—C12—C13	−2.6 (2)
C2—C3—C4—C5	−0.33 (17)	C17—C11—C12—C13	177.24 (13)
C37—C3—C4—C5	179.11 (12)	C11—C12—C13—C14	−0.1 (2)
C3—C4—C5—S1	0.29 (15)	C12—C13—C14—C15	2.5 (2)
C2—S1—C5—C4	−0.14 (11)	C12—C13—C14—C141	−178.03 (13)
C2—C3—C37—C17	176.17 (13)	C13—C14—C15—C16	−2.1 (2)

C4—C3—C37—C17	−3.2 (2)	C141—C14—C15—C16	178.38 (13)
C2—C3—C37—C371	0.06 (18)	C14—C15—C16—C11	−0.6 (2)
C4—C3—C37—C371	−179.31 (12)	C12—C11—C16—C15	2.9 (2)
C371—C37—C17—C11	−2.1 (2)	C17—C11—C16—C15	−176.91 (13)
C3—C37—C17—C11	−177.98 (12)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N37^{i}	0.95	2.75	3.312 (2)	119
C13—H13···*Cg*^{ii}	0.95	2.99	3.777 (2)	141

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) *x*, −*y*−1/2, *z*−1/2.