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(*E*)-2-(2-Anilinovinyl)-3,4-dimethylthiazol-3-ium iodide

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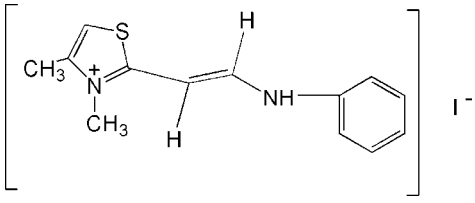
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.031; wR factor = 0.084; data-to-parameter ratio = 19.9.

In the title compound, $C_{13}H_{15}N_2S^+\cdot I^-$, the organic cation is almost planar and the N atoms have nearly trigonal-planar geometry. The crystal packing involves N—H···I hydrogen bonds, aromatic π–π stacking [centroid-to-centroid separation 3.631 (2) Å; symmetry code: $-x+1, -y, -z+1$], a C—H···π interaction and a weak S···I interaction [3.7645 (11) Å; symmetry code: $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$].

Related literature

The title compound was synthesized by a literature method (Hung *et al.*, 1996; Li & Peng, 1995; Boto *et al.*, 2007). For structural analogues, see: Sax *et al.* (1974); Kluger *et al.* (1987).



Experimental

Crystal data

$C_{13}H_{15}N_2S^+\cdot I^-$
M_r = 358.24
Monoclinic, $C2/c$
a = 15.830 (3) Å
b = 11.3918 (15) Å
c = 16.787 (3) Å
β = 114.118 (11)°
V = 2763.0 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.45 mm^{-1}
T = 295 (2) K
0.21 × 0.18 × 0.11 mm

Data collection

Bruker $P4$ diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.602, T_{max} = 0.760
3886 measured reflections
3185 independent reflections
2530 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
7 standard reflections
every 99 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.084
S = 1.03
3185 reflections
160 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

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

Cg is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*A*···I1	0.81 (3)	2.77 (3)	3.573 (3)	174 (3)
C12—H12*A*···*Cg*^{i}	0.96	2.76	–	–

Symmetry code: (i) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+1$.

Data collection: *XSCANS* (Bruker, 1998); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2497).

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supplementary materials

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(*E*)-2-(2-Anilinovinyl)-3,4-dimethylthiazol-3-ium iodide

C.-H. Ge, Z.-J. Guo, G. Yanan, W. Guan and X.-D. Zhang

Comment

As part of our studies of cyanine related dyes, the title compound, (I), (Fig. 1) was obtained as the product of reaction of 2,3,4-trimethyl-thiazol-3-ium iodide, aniline and triethyl orthoformiate. The atoms of the organic molecule (except H12A–H12C/H13A–H13C) are nearly coplanar with the largest deviation of 0.0846 Å for N2. The sum of the bond angles of the quaternary N2 atom is 360.0°. The N1—C7 bond distance of 1.340 (4)Å is indicative of strong π-conjugation.

The crystal packing (Fig. 2) features a π–π stacking interaction with a centroid separation $Cg\cdots Cg^{i}$ (i = 1 − *x*, −*y*, 1 − *z*) = 3.631 (2) Å and a C—H···π interaction with H12A···*Cg* (ii = 3/2 − *x*, 1/2 − *y*, 1 − *z*) = 2.76 Å (*Cg* is the ring centroid defined by atoms C1–C6) generate a supramolecular framework with [001] channels.

The I^{-} counter ions are fixed in these channels by means of an N—H···I hydrogen bond (Table 1) and weak S···I interactions [$S1\cdots I1^{iii}$ (iii = 1/2 − *x*, −1/2 + *y*, 1/2 − *z*) = 3.7645 (11) Å].

Experimental

The title compound was prepared by the method of Boto *et al.* (2007). Red blocks of (I) were recrystallized from dry methanol/diethyl ether.

Refinement

The H atoms were located in a difference map but those attached to C atoms were repositioned geometrically. Their positions were refined, initially with restraints, and then as riding, resulting in C—H distances in the range 0.93–1.00 Å and N—H = 0.81–0.84 Å).

Figures

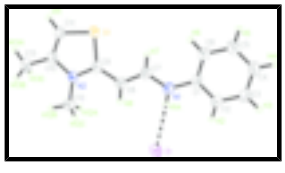


Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms). The hydrogen bond is indicated as dashed line.

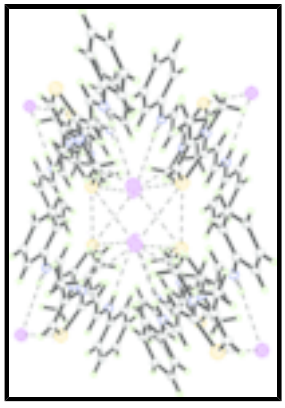


Fig. 2. Fragment of (I) along the *c* diraction, showing that the I^- ions are trapped within the [001] channels.

(*E*)-2-(2-Anilinovinyl)-3,4-dimethylthiazol-3-ium iodide

Crystal data

$C_{13}H_{15}N_2S^+\cdot I^-$	F_{000} = 1408
M_r = 358.24	D_x = 1.722 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C2yc	Cell parameters from 842 reflections
a = 15.830 (3) Å	θ = 2.7–22.5º
b = 11.3918 (15) Å	μ = 2.45 mm^{-1}
c = 16.787 (3) Å	*T* = 295 (2) K
β = 114.118 (11)º	Block, red
V = 2763.0 (8) Å^3	0.21 × 0.18 × 0.11 mm
Z = 8	

Data collection

Bruker P4 diffractometer	R_{int} = 0.033
Radiation source: fine-focus sealed tube	θ_{max} = 27.5º
Monochromator: graphite	θ_{min} = 2.3º
T = 295(2) K	*h* = −20→1
ω scans	*k* = −14→1
Absorption correction: multi-scan (SADABS; Bruker, 1999)	*l* = −20→21
T_{min} = 0.602, T_{max} = 0.760	7 standard reflections
3886 measured reflections	every 99 reflections
3185 independent reflections	intensity decay: none
2530 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.084$	$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 2.2252P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
3185 reflections	$\Delta\rho_{max} = 0.98$ e Å^{-3}
160 parameters	$\Delta\rho_{min} = -0.88$ 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}
I1	0.910963 (14)	0.004448 (18)	0.580356 (13)	0.04055 (9)
S1	0.60582 (5)	0.30762 (7)	0.23224 (5)	0.03483 (17)
N2	0.75770 (15)	0.2168 (2)	0.24803 (14)	0.0307 (5)
C8	0.7179 (2)	0.1634 (3)	0.36907 (18)	0.0342 (6)
H8	0.7731	0.1220	0.3955	0.041*
C7	0.6589 (2)	0.1649 (2)	0.40926 (18)	0.0333 (6)
H7	0.6023	0.2029	0.3819	0.040*
C11	0.6462 (2)	0.3346 (3)	0.15299 (18)	0.0343 (6)
H11	0.6147	0.3797	0.1035	0.041*
N1	0.67922 (19)	0.1137 (2)	0.48681 (16)	0.0366 (6)
C10	0.7276 (2)	0.2835 (3)	0.17069 (18)	0.0329 (6)
C6	0.5398 (2)	0.1630 (3)	0.5086 (2)	0.0418 (7)
H6	0.5172	0.2079	0.4579	0.050*
C9	0.70041 (19)	0.2212 (2)	0.28914 (18)	0.0300 (6)
C2	0.6599 (2)	0.0458 (3)	0.61312 (19)	0.0382 (7)
H2	0.7181	0.0112	0.6324	0.046*
C1	0.6249 (2)	0.1085 (2)	0.53502 (17)	0.0318 (6)
C3	0.6082 (3)	0.0355 (3)	0.6613 (2)	0.0441 (8)
H3	0.6315	−0.0070	0.7132	0.053*
C5	0.4884 (2)	0.1506 (3)	0.5578 (2)	0.0480 (8)
H5	0.4304	0.1857	0.5391	0.058*
C13	0.7850 (3)	0.2912 (3)	0.1196 (2)	0.0480 (8)
H13A	0.7552	0.3418	0.0703	0.072*

H13B	0.7920	0.2143	0.0997	0.072*
H13C	0.8448	0.3224	0.1558	0.072*
C4	0.5222 (2)	0.0870 (3)	0.6340 (2)	0.0459 (8)
H4	0.4874	0.0788	0.6668	0.055*
C12	0.8446 (2)	0.1497 (3)	0.2817 (2)	0.0431 (7)
H12A	0.8873	0.1849	0.3349	0.065*
H12B	0.8709	0.1501	0.2393	0.065*
H12C	0.8323	0.0703	0.2929	0.065*
H1A	0.730 (2)	0.084 (3)	0.508 (2)	0.043 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.03565 (13)	0.04473 (14)	0.04291 (14)	−0.00040 (9)	0.01772 (10)	−0.00322 (9)
S1	0.0328 (4)	0.0414 (4)	0.0344 (4)	0.0038 (3)	0.0180 (3)	0.0021 (3)
N2	0.0331 (12)	0.0329 (11)	0.0295 (11)	0.0014 (10)	0.0162 (10)	−0.0025 (10)
C8	0.0366 (15)	0.0361 (15)	0.0294 (14)	0.0005 (12)	0.0131 (12)	0.0009 (12)
C7	0.0375 (15)	0.0322 (14)	0.0294 (13)	−0.0008 (12)	0.0131 (12)	0.0004 (11)
C11	0.0396 (15)	0.0382 (15)	0.0270 (13)	0.0002 (13)	0.0156 (12)	0.0014 (12)
N1	0.0366 (14)	0.0436 (15)	0.0316 (13)	0.0041 (12)	0.0159 (11)	0.0082 (11)
C10	0.0392 (15)	0.0350 (15)	0.0295 (13)	−0.0013 (12)	0.0190 (12)	−0.0021 (12)
C6	0.0433 (17)	0.0486 (19)	0.0360 (16)	0.0078 (15)	0.0188 (13)	0.0118 (14)
C9	0.0325 (14)	0.0299 (14)	0.0304 (13)	−0.0036 (12)	0.0157 (11)	−0.0032 (11)
C2	0.0413 (17)	0.0407 (16)	0.0338 (15)	0.0073 (14)	0.0165 (13)	0.0076 (13)
C1	0.0377 (15)	0.0317 (14)	0.0290 (13)	−0.0028 (12)	0.0166 (12)	0.0007 (11)
C3	0.060 (2)	0.0401 (16)	0.0375 (16)	0.0022 (16)	0.0259 (16)	0.0082 (14)
C5	0.0415 (18)	0.062 (2)	0.0450 (18)	0.0098 (16)	0.0221 (15)	0.0058 (17)
C13	0.056 (2)	0.057 (2)	0.0435 (17)	0.0092 (17)	0.0337 (16)	0.0060 (16)
C4	0.052 (2)	0.053 (2)	0.0429 (17)	−0.0006 (16)	0.0297 (16)	0.0013 (16)
C12	0.0392 (16)	0.0488 (18)	0.0427 (18)	0.0097 (15)	0.0182 (14)	0.0037 (15)

Geometric parameters (Å, °)

S1—C9	1.719 (3)	C6—C5	1.384 (4)
S1—C11	1.722 (3)	C6—H6	0.9300
N2—C9	1.346 (3)	C2—C3	1.371 (5)
N2—C10	1.408 (3)	C2—C1	1.393 (4)
N2—C12	1.470 (4)	C2—H2	0.9300
C8—C7	1.358 (4)	C3—C4	1.377 (5)
C8—C9	1.417 (4)	C3—H3	0.9300
C8—H8	0.9300	C5—C4	1.374 (5)
C7—N1	1.340 (4)	C5—H5	0.9300
C7—H7	0.9300	C13—H13A	0.9600
C11—C10	1.333 (4)	C13—H13B	0.9600
C11—H11	0.9300	C13—H13C	0.9600
N1—C1	1.403 (4)	C4—H4	0.9300
N1—H1A	0.81 (3)	C12—H12A	0.9600
C10—C13	1.485 (4)	C12—H12B	0.9600
C6—C1	1.381 (4)	C12—H12C	0.9600

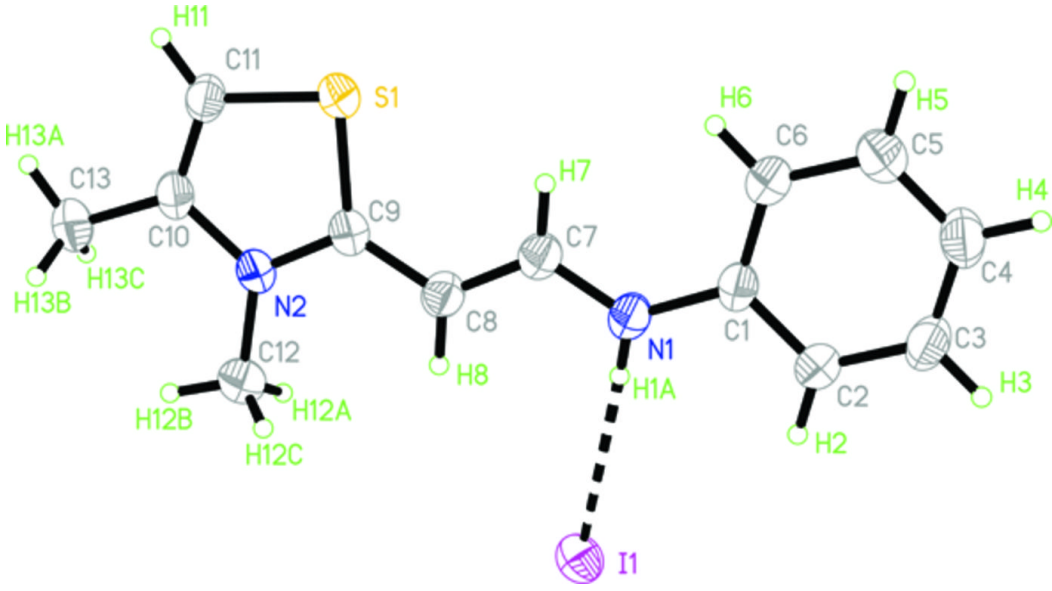
C9—S1—C11	91.02 (14)	C3—C2—H2	120.2
C9—N2—C10	114.0 (2)	C1—C2—H2	120.2
C9—N2—C12	122.9 (2)	C6—C1—C2	119.6 (3)
C10—N2—C12	123.1 (2)	C6—C1—N1	122.9 (3)
C7—C8—C9	123.8 (3)	C2—C1—N1	117.5 (3)
C7—C8—H8	118.1	C2—C3—C4	120.9 (3)
C9—C8—H8	118.1	C2—C3—H3	119.6
N1—C7—C8	122.5 (3)	C4—C3—H3	119.6
N1—C7—H7	118.8	C4—C5—C6	120.6 (3)
C8—C7—H7	118.8	C4—C5—H5	119.7
C10—C11—S1	112.3 (2)	C6—C5—H5	119.7
C10—C11—H11	123.8	C10—C13—H13A	109.5
S1—C11—H11	123.8	C10—C13—H13B	109.5
C7—N1—C1	128.2 (3)	H13A—C13—H13B	109.5
C7—N1—H1A	114 (2)	C10—C13—H13C	109.5
C1—N1—H1A	118 (2)	H13A—C13—H13C	109.5
C11—C10—N2	111.9 (2)	H13B—C13—H13C	109.5
C11—C10—C13	127.6 (3)	C5—C4—C3	119.4 (3)
N2—C10—C13	120.5 (3)	C5—C4—H4	120.3
C1—C6—C5	119.7 (3)	C3—C4—H4	120.3
C1—C6—H6	120.1	N2—C12—H12A	109.5
C5—C6—H6	120.1	N2—C12—H12B	109.5
N2—C9—C8	123.8 (3)	H12A—C12—H12B	109.5
N2—C9—S1	110.7 (2)	N2—C12—H12C	109.5
C8—C9—S1	125.6 (2)	H12A—C12—H12C	109.5
C3—C2—C1	119.7 (3)	H12B—C12—H12C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···I1	0.81 (3)	2.77 (3)	3.573 (3)	174 (3)
C12—H12A···Cg^{i}	0.96	2.76	Missing	Missing

Symmetry codes: (i) −*x*+3/2, −*y*+1/2, −*z*+1.

Fig. 1


H11
C11
S1
H13A
C13
C10
C9
H7
C7
H6
C6
H5
C5
H4
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H13B
N2
C8
N1
C1
C3
H3
C12
H8
H1A
C2
H12B
H12A
H2
H12C
I1

Fig. 2