Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-[(*E*)-2-(4-Methoxyphenyl)ethenyl]-1-methylpyridinium iodide

K. Senthil,[a] S. Kalainathan,[a] A. RubanKumar,[a] V. Ramkumar[b] and Jiban Podder[c]*

[a]Centre for Crystal Growth, School of Advanced Sciences, VIT University, Vellore, Tamil Nadu, India, [b]Department of Chemistry, IIT Madras, Chennai 600 036, TamilNadu, India, and [c]Department of Physics, Bangladesh University of Engineering and Technology, Dhaka 1000, Bangladesh
Correspondence e-mail: jpodder59@gmail.com

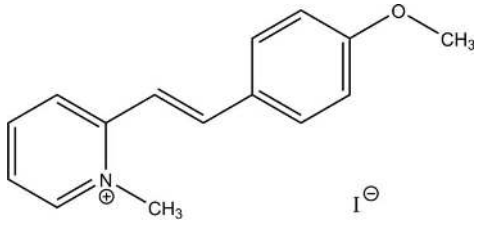
Received 13 November 2013; accepted 22 November 2013

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.020; wR factor = 0.052; data-to-parameter ratio = 15.0.

In the title molecular salt, $C_{16}H_{10}NO^{+}\cdot I^{-}$, the dihedral angle between the pyridinium and benzene rings is 6.61 (8)°. In the crystal, the cation is linked to the anion by a C—H···I interaction arising from the activated aromatic C atom adjacent to the N^{+} cation.

Related literature

For background to organic non-linear optical materials, see: Jagannathan *et al.* (2007); Williams (1984). For a related structure, see: Chantrapromma *et al.* (2010).



Experimental

Crystal data

$C_{15}H_{16}NO^{+}\cdot I^{-}$
M_r = 353.19
Triclinic, $P\overline{1}$
a = 7.1760 (3) Å
b = 8.6895 (4) Å
c = 12.1555 (6) Å
α = 92.645 (2)°
β = 92.115 (2)°
γ = 103.781 (2)°
V = 734.47 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.17 mm^{-1}
T = 298 K
0.25 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.613, T_{max} = 0.737
8523 measured reflections
2470 independent reflections
2363 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.052
S = 1.09
2470 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···I1^{i}	0.93	2.96	3.872 (3)	168

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97*.

The authors thank the DRDO, Government of India, for financial support. They also thank the VIT University management, Vellore, for their constant support and encouragement and acknowledge the Department of Chemistry, IIT Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7162).

References

Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chantrapromma, S., Chanawanno, K. & Fun, H.-K. (2010). *Acta Cryst.* E**66**, o1975–o1976.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Jagannathan, K., Kalainathan, S., Gnanasekaran, T., Vijayan, N. & Bhagavannarayana, G. (2007). *Cryst. Res. Technol.* **42**, 483–487.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Williams, D. J. (1984). *Angew. Chem. Int. Ed. Engl.* **23**, 690–703.

supporting information

Acta Cryst. (2013). E**69**, o1848 [doi:10.1107/S1600536813031929]

2-[(*E*)-2-(4-Methoxyphenyl)ethenyl]-1-methylpyridinium iodide

K. Senthil, S. Kalainathan, A. RubanKumar, V. Ramkumar and Jiban Podder

S1. Comment

In recent years, the design of new organic nonlinear optical (NLO) materials have been studied (e.g. Jagannathan *et al.*, 2007). As part of our stuies in this area, the title pyridinium derivative compound was synthesized,. It crystallizes in the centrosymmetric Pī triclinic space group, so it does not exhibit second-order nonlinear optical properties (Williams, 1984).

The cation is essentially planar and exist in E configuration. The dihedral angle between the pyridinium and benzene rings is 6.16 (8)°. Bond lengths and angles are comparable with those for closely related structure (Chantrapromma *et al.*, 2010). In the crystal, the cation is linked to the anion by a C—H···I interaction (Table 1).

S2. Experimental

The title compound was prepared by mixing 1:1 molar ratio of solutions of 1,2-dimethylpyridinium iodide (7.052 g, 30 mmol), 4-methoxy benzaldehyde (3.7 ml, 30 mmol) and piperidine (5 drops) in hot methanol (20 ml). The resulting mixture was refluxed at 60°C for 8 h to give yellowish crystalline product, which was filtered off and washed with di-ethyl ether and dried. Yellow needle-shaped single crystals of the title compound suitable for X-ray structure determination were obtained by recrystallization (three times) from methanol–acetonitrile (1:1) mixture by slow evaporation of the solvent at ambient temperature over several days (m.p. 514–516 K).

S3. Refinement

All hydrogen atoms were fixed geometrically (C—H 0.93–0.98 Å) and refined as riding, with U_{iso}(H) = 1.2–1.5 U_{eq}(C).

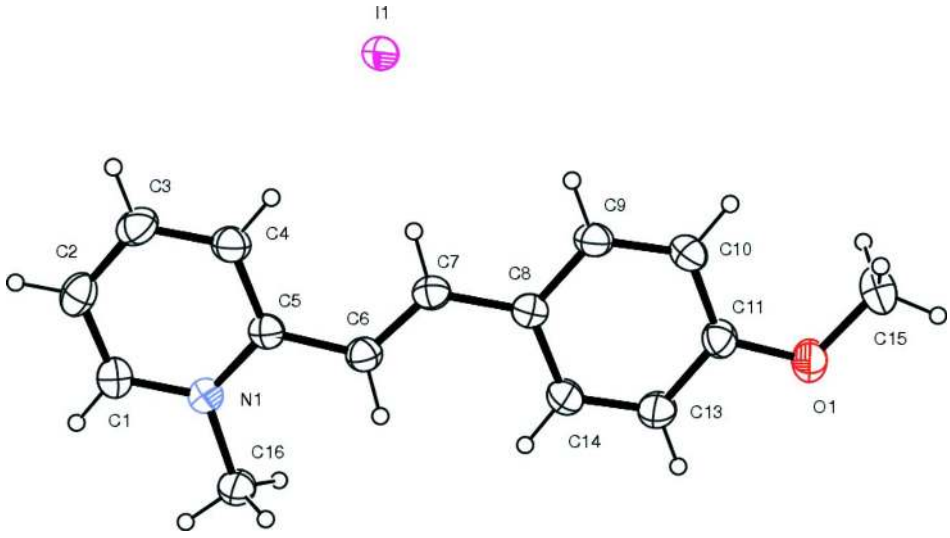


Figure 1

ORTEP of the molecule with atoms represented as 30% probability ellipsoids.

2-[(*E*)-2-(4-Methoxyphenyl)ethenyl]-1-methylpyridinium iodide

Crystal data

$C_{15}H_{16}NO^{+}\cdot I^{-}$
$M_r = 353.19$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.1760\ (3)$ Å
$b = 8.6895\ (4)$ Å
$c = 12.1555\ (6)$ Å
$\alpha = 92.645\ (2)°$
$\beta = 92.115\ (2)°$
$\gamma = 103.781\ (2)°$
$V = 734.47\ (6)$ Å^3
$Z = 2$
$F(000) = 348$
$D_x = 1.597$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8234 reflections
$\theta = 2.4–28.4°$
$\mu = 2.17$ mm^{-1}
$T = 298$ K
Slab, yellow
0.25 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.613$, $T_{max} = 0.737$
8523 measured reflections
2470 independent reflections
2363 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -8\rightarrow6$
$k = -10\rightarrow10$
$l = -12\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.052$
$S = 1.09$
2470 reflections
165 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

$w = 1/[\sigma^2(F_o^2) + (0.0211P)^2 + 0.414P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0288 (14)

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 $F^2 > \sigma(F^2)$ 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}
C1	−0.1445 (4)	0.0480 (3)	0.8878 (2)	0.0494 (6)
H1	−0.2582	−0.0296	0.8742	0.059*
C2	−0.1376 (4)	0.1673 (3)	0.9651 (2)	0.0560 (7)
H2	−0.2451	0.1722	1.0043	0.067*
C3	0.0321 (5)	0.2809 (3)	0.9843 (2)	0.0598 (7)
H3	0.0397	0.3633	1.0372	0.072*
C4	0.1896 (4)	0.2736 (3)	0.9260 (2)	0.0537 (6)
H4	0.3039	0.3503	0.9400	0.064*
C5	0.1799 (4)	0.1513 (3)	0.84555 (19)	0.0419 (5)
C6	0.3386 (4)	0.1382 (3)	0.7790 (2)	0.0468 (6)
H6	0.3297	0.0432	0.7383	0.056*
C7	0.4961 (4)	0.2531 (3)	0.7722 (2)	0.0460 (5)
H7	0.5055	0.3449	0.8167	0.055*
C8	0.6550 (3)	0.2503 (3)	0.7027 (2)	0.0422 (5)
C9	0.8189 (4)	0.3743 (3)	0.7121 (2)	0.0497 (6)
H9	0.8233	0.4583	0.7632	0.060*
C10	0.9754 (4)	0.3779 (3)	0.6488 (2)	0.0497 (6)
H10	1.0838	0.4618	0.6580	0.060*
C11	0.9687 (4)	0.2554 (3)	0.5718 (2)	0.0497 (6)
C13	0.8062 (4)	0.1296 (3)	0.5607 (3)	0.0622 (7)
H13	0.8019	0.0465	0.5088	0.075*
C14	0.6536 (4)	0.1264 (3)	0.6246 (2)	0.0549 (6)
H14	0.5470	0.0408	0.6163	0.066*
C15	1.2825 (4)	0.3695 (4)	0.5113 (3)	0.0652 (8)
H15A	1.2501	0.4670	0.4943	0.098*
H15B	1.3708	0.3459	0.4594	0.098*
H15C	1.3410	0.3800	0.5845	0.098*
C16	−0.0104 (4)	−0.0956 (3)	0.7487 (2)	0.0561 (7)
H16A	−0.1383	−0.1617	0.7491	0.084*
H16B	0.0805	−0.1563	0.7676	0.084*
H16C	0.0128	−0.0567	0.6766	0.084*

N1	0.0107 (3)	0.0400 (2)	0.83019 (16)	0.0409 (4)
O1	1.1126 (3)	0.2441 (3)	0.50511 (19)	0.0726 (6)
I1	0.43035 (2)	0.689767 (18)	0.803640 (16)	0.05847 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0449 (13)	0.0580 (14)	0.0471 (14)	0.0149 (11)	0.0023 (11)	0.0090 (11)
C2	0.0638 (17)	0.0679 (16)	0.0428 (14)	0.0267 (14)	0.0105 (12)	0.0086 (12)
C3	0.085 (2)	0.0533 (15)	0.0434 (14)	0.0208 (14)	0.0134 (14)	0.0002 (11)
C4	0.0653 (16)	0.0454 (13)	0.0461 (14)	0.0048 (12)	0.0071 (12)	0.0004 (11)
C5	0.0502 (13)	0.0407 (11)	0.0355 (12)	0.0111 (10)	0.0015 (10)	0.0082 (9)
C6	0.0512 (14)	0.0437 (12)	0.0445 (13)	0.0096 (11)	0.0032 (11)	−0.0003 (10)
C7	0.0524 (14)	0.0402 (12)	0.0460 (14)	0.0123 (10)	0.0012 (11)	0.0025 (10)
C8	0.0435 (12)	0.0410 (11)	0.0425 (13)	0.0114 (10)	−0.0032 (10)	0.0045 (9)
C9	0.0563 (15)	0.0415 (12)	0.0475 (14)	0.0053 (11)	0.0016 (12)	−0.0025 (10)
C10	0.0460 (13)	0.0471 (13)	0.0510 (15)	0.0022 (10)	−0.0012 (11)	0.0014 (11)
C11	0.0401 (13)	0.0570 (14)	0.0507 (15)	0.0100 (11)	−0.0010 (11)	−0.0012 (11)
C13	0.0506 (15)	0.0616 (16)	0.0677 (19)	0.0053 (13)	0.0024 (13)	−0.0226 (14)
C14	0.0422 (13)	0.0537 (14)	0.0620 (17)	0.0012 (11)	−0.0002 (12)	−0.0104 (12)
C15	0.0443 (15)	0.0802 (19)	0.0671 (19)	0.0053 (14)	0.0059 (13)	0.0111 (15)
C16	0.0487 (14)	0.0548 (14)	0.0596 (17)	0.0057 (12)	0.0012 (12)	−0.0122 (12)
N1	0.0442 (11)	0.0444 (10)	0.0349 (10)	0.0125 (8)	−0.0016 (8)	0.0045 (8)
O1	0.0491 (11)	0.0816 (14)	0.0795 (15)	0.0041 (10)	0.0153 (10)	−0.0219 (11)
I1	0.04875 (13)	0.04564 (12)	0.07815 (17)	0.00721 (8)	0.00877 (9)	−0.00920 (8)

Geometric parameters (Å, º)

C1—N1	1.351 (3)	C9—C10	1.380 (4)
C1—C2	1.357 (4)	C9—H9	0.9300
C1—H1	0.9300	C10—C11	1.375 (4)
C2—C3	1.377 (4)	C10—H10	0.9300
C2—H2	0.9300	C11—O1	1.355 (3)
C3—C4	1.369 (4)	C11—C13	1.393 (4)
C3—H3	0.9300	C13—C14	1.362 (4)
C4—C5	1.397 (4)	C13—H13	0.9300
C4—H4	0.9300	C14—H14	0.9300
C5—N1	1.361 (3)	C15—O1	1.426 (3)
C5—C6	1.445 (3)	C15—H15A	0.9600
C6—C7	1.326 (4)	C15—H15B	0.9600
C6—H6	0.9300	C15—H15C	0.9600
C7—C8	1.448 (4)	C16—N1	1.479 (3)
C7—H7	0.9300	C16—H16A	0.9600
C8—C9	1.390 (3)	C16—H16B	0.9600
C8—C14	1.400 (4)	C16—H16C	0.9600
N1—C1—C2	121.2 (2)	C11—C10—H10	120.5
N1—C1—H1	119.4	C9—C10—H10	120.5

C2—C1—H1	119.4	O1—C11—C10	124.9 (2)
C1—C2—C3	118.6 (3)	O1—C11—C13	115.6 (2)
C1—C2—H2	120.7	C10—C11—C13	119.5 (2)
C3—C2—H2	120.7	C14—C13—C11	121.0 (3)
C4—C3—C2	120.5 (3)	C14—C13—H13	119.5
C4—C3—H3	119.8	C11—C13—H13	119.5
C2—C3—H3	119.8	C13—C14—C8	120.9 (2)
C3—C4—C5	120.4 (3)	C13—C14—H14	119.6
C3—C4—H4	119.8	C8—C14—H14	119.6
C5—C4—H4	119.8	O1—C15—H15A	109.5
N1—C5—C4	117.4 (2)	O1—C15—H15B	109.5
N1—C5—C6	119.1 (2)	H15A—C15—H15B	109.5
C4—C5—C6	123.5 (2)	O1—C15—H15C	109.5
C7—C6—C5	124.1 (2)	H15A—C15—H15C	109.5
C7—C6—H6	117.9	H15B—C15—H15C	109.5
C5—C6—H6	117.9	N1—C16—H16A	109.5
C6—C7—C8	126.7 (2)	N1—C16—H16B	109.5
C6—C7—H7	116.6	H16A—C16—H16B	109.5
C8—C7—H7	116.6	N1—C16—H16C	109.5
C9—C8—C14	117.0 (2)	H16A—C16—H16C	109.5
C9—C8—C7	120.0 (2)	H16B—C16—H16C	109.5
C14—C8—C7	123.0 (2)	C1—N1—C5	121.9 (2)
C10—C9—C8	122.7 (2)	C1—N1—C16	117.2 (2)
C10—C9—H9	118.7	C5—N1—C16	120.9 (2)
C8—C9—H9	118.7	C11—O1—C15	118.6 (2)
C11—C10—C9	119.0 (2)		

N1—C1—C2—C3	−0.2 (4)	C9—C10—C11—C13	−1.1 (4)
C1—C2—C3—C4	0.3 (4)	O1—C11—C13—C14	178.9 (3)
C2—C3—C4—C5	0.6 (4)	C10—C11—C13—C14	0.2 (5)
C3—C4—C5—N1	−1.5 (4)	C11—C13—C14—C8	0.6 (5)
C3—C4—C5—C6	178.4 (2)	C9—C8—C14—C13	−0.6 (4)
N1—C5—C6—C7	167.1 (2)	C7—C8—C14—C13	179.6 (3)
C4—C5—C6—C7	−12.8 (4)	C2—C1—N1—C5	−0.9 (4)
C5—C6—C7—C8	−176.5 (2)	C2—C1—N1—C16	179.3 (2)
C6—C7—C8—C9	−174.0 (3)	C4—C5—N1—C1	1.7 (3)
C6—C7—C8—C14	5.8 (4)	C6—C5—N1—C1	−178.2 (2)
C14—C8—C9—C10	−0.2 (4)	C4—C5—N1—C16	−178.4 (2)
C7—C8—C9—C10	179.5 (2)	C6—C5—N1—C16	1.6 (3)
C8—C9—C10—C11	1.1 (4)	C10—C11—O1—C15	−2.1 (4)
C9—C10—C11—O1	−179.6 (3)	C13—C11—O1—C15	179.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···I1^{i}	0.93	2.96	3.872 (3)	168

Symmetry code: (i) *x*−1, *y*−1, *z*.