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## Structure Reports

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## 4-Methoxyanilinium iodide

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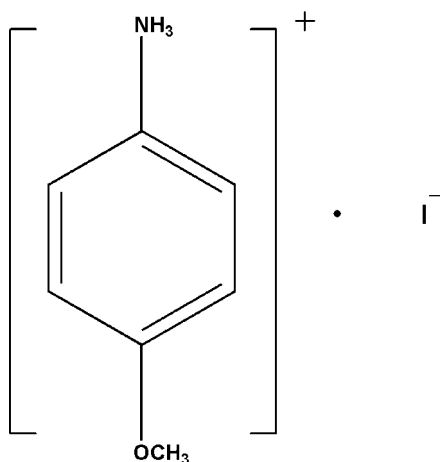
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.032;  $wR$  factor = 0.065; data-to-parameter ratio = 19.6.

The crystal structure of the title compound,  $\text{C}_7\text{H}_{10}\text{NO}^+\cdot\text{I}^-$ , displays  $\text{N}-\text{H}\cdots\text{I}$  hydrogen bonds between the 4-methoxyanilinium cations and the iodide anion together with weaker  $\text{C}-\text{H}\cdots\pi$  contacts.

## Related literature

The title compound was investigated as a potential candidate for having good dielectric properties. For compounds with dielectric-ferroelectric properties, see: Hang *et al.* (2009); Li *et al.* (2008).



## Experimental

## Crystal data

 $\text{C}_7\text{H}_{10}\text{NO}^+\cdot\text{I}^-$  $M_r = 251.06$ Orthorhombic,  $Pbca$ 

$a = 12.290$  (3) Å  
 $b = 7.1302$  (14) Å  
 $c = 20.304$  (4) Å  
 $V = 1779.2$  (6) Å<sup>3</sup>

 $Z = 8$ Mo  $K\alpha$  radiation $\mu = 3.54$  mm<sup>-1</sup> $T = 298$  K $0.40 \times 0.30 \times 0.20$  mm

## Data collection

Rigaku SCXmini diffractometer  
Absorption correction: multi-scan  
(*CrystalClear*; Rigaku, 2005)  
 $T_{\min} = 0.291$ ,  $T_{\max} = 0.493$

16921 measured reflections  
2040 independent reflections  
1803 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.052$

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.032$  $wR(F^2) = 0.065$  $S = 1.25$ 

2040 reflections

104 parameters

3 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.51$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.45$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C2–C7 ring.

| $D-H\cdots A$                                      | $D-H$    | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------------------------|----------|-------------|-------------|---------------|
| $\text{N1}-\text{H1D}\cdots\text{I1}^{\text{i}}$   | 0.86 (3) | 2.67 (2)    | 3.503 (3)   | 165 (5)       |
| $\text{N1}-\text{H1F}\cdots\text{I1}^{\text{ii}}$  | 0.86 (1) | 2.75 (2)    | 3.566 (3)   | 159 (3)       |
| $\text{N1}-\text{H1E}\cdots\text{I1}$              | 0.86 (4) | 2.75 (4)    | 3.568 (3)   | 159 (4)       |
| $\text{C4}-\text{H4}\cdots\text{Cg1}^{\text{iii}}$ | 0.93     | 2.87        | 3.627 (4)   | 140           |
| $\text{C7}-\text{H7}\cdots\text{Cg1}^{\text{iv}}$  | 0.93     | 2.62        | 3.483 (4)   | 155           |

Symmetry codes: (i)  $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$ ; (ii)  $-x + 1, -y + 1, -z + 1$ ; (iii)  $-x + \frac{1}{2}, y + \frac{1}{2}, z$ ; (iv)  $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$ .

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The author thanks Southeast University for financial support of this research and is very grateful for the guidance of Professor Wen Zhang.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2356).

## References

- Hang, T., Fu, D. W., Ye, Q. & Xiong, R. G. (2009). *Cryst. Growth Des.* **5**, 2026–2029.  
Li, X. Z., Qu, Z. R. & Xiong, R. G. (2008). *Chin. J. Chem.* **11**, 1959–1962.  
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## supporting information

*Acta Cryst.* (2010). E66, o3316 [https://doi.org/10.1107/S1600536810047549]

## 4-Methoxyanilinium iodide

Rui-jun Xu

## S1. Comment

Dielectric-ferroelectric constitute an interesting class of materials, comprising organic ligands (Li *et al.*, 2008), metal-organic coordination compounds (Hang *et al.*, 2009) and organic-inorganic hybrids. We were interested in the title compound as a potential candidate for having good dielectric properties. Unfortunately, the capacitance and dielectric loss measurements did not show any distinct anomaly when observed from 93 K to 455 K (its sublimation temperature). Regarding its crystal structure, the asymmetric unit of the title compound contains a (4-methoxyanilinium) cation and a iodide anion (Fig.1). The structure is stabilized by C—H $\cdots$  $\pi$  interactions (C4—H4 $\cdots$ Cg1 3.627 (4) Å and C7—H7 $\cdots$ Cg1 3.483 (4) Å) as well as weak N—H $\cdots$ I hydrogen bonds involving the NH<sub>3</sub> group and linking the cations and anions into a 3D structure (Fig. 2 and Tab. 1).

## S2. Experimental

The title compound was obtained by the addition of hydriodic acid (4.12 ml, 0.022 mol) to a solution of 4-methoxyanilin (2.26 g, 0.02 mol) in ethanol, in the stoichiometric ratio 1.1:1. Good quality single crystals were obtained by slow evaporation after two weeks.

## S3. Refinement

Positional parameters of all the H atoms were calculated geometrically and the H atoms were set to ride on the C and N atoms to which they are bonded, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C or N})$ .

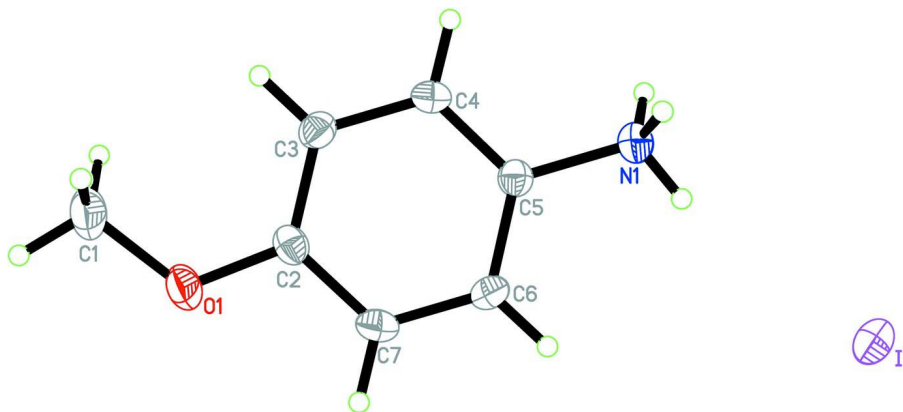


Figure 1

The molecular structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

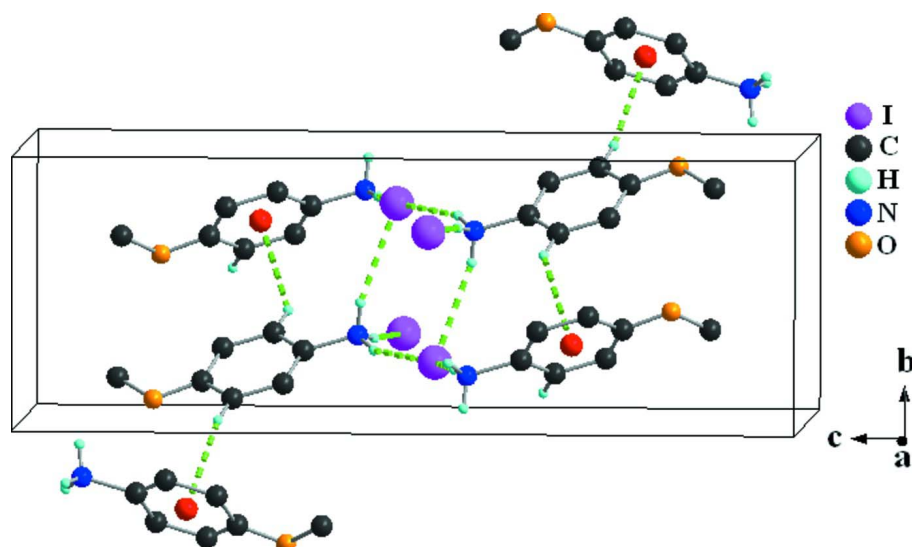


Figure 2

A view of the packing of the title compound, stacking along the *b* axis. Dashed lines indicate hydrogen bonds.

#### 4-Methoxyanilinium iodide

##### Crystal data

$C_7H_{10}NO^+ \cdot I^-$

$M_r = 251.06$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 12.290$  (3) Å

$b = 7.1302$  (14) Å

$c = 20.304$  (4) Å

$V = 1779.2$  (6) Å<sup>3</sup>

$Z = 8$

$F(000) = 960$

$D_x = 1.875$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 7161 reflections

$\theta = 3.0$ – $27.7^\circ$

$\mu = 3.54$  mm<sup>-1</sup>

$T = 298$  K

Prism, colourless

$0.40 \times 0.30 \times 0.20$  mm

##### Data collection

Rigaku SCXmini  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 13.6612 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan

(*CrystalClear*; Rigaku, 2005)

$T_{\min} = 0.291$ ,  $T_{\max} = 0.493$

16921 measured reflections

2040 independent reflections

1803 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$

$\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.3^\circ$

$h = -15 \rightarrow 15$

$k = -9 \rightarrow 9$

$l = -26 \rightarrow 26$

##### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.065$

$S = 1.25$

2040 reflections

104 parameters

3 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

H atoms treated by a mixture of independent  
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0154P)^2 + 1.2835P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.51 \text{ e } \text{Å}^{-3}$

$$\Delta\rho_{\min} = -0.45 \text{ e } \text{Å}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick, 2008),  $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0053 (2)

*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<sup>2</sup>)*

|     | <i>x</i>      | <i>y</i>    | <i>z</i>      | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|-------------|---------------|----------------------------------|
| I1  | 0.613461 (19) | 0.22260 (3) | 0.471872 (12) | 0.04311 (12)                     |
| C1  | 0.3182 (4)    | 0.1321 (6)  | 0.88673 (18)  | 0.0580 (11)                      |
| H1A | 0.3321        | 0.0724      | 0.9283        | 0.087*                           |
| H1B | 0.2444        | 0.1083      | 0.8736        | 0.087*                           |
| H1C | 0.3293        | 0.2648      | 0.8909        | 0.087*                           |
| C2  | 0.3836 (3)    | 0.1268 (4)  | 0.77653 (15)  | 0.0332 (7)                       |
| C3  | 0.3010 (3)    | 0.2400 (4)  | 0.75290 (18)  | 0.0347 (7)                       |
| H3  | 0.2448        | 0.2778      | 0.7806        | 0.042*                           |
| C4  | 0.3024 (3)    | 0.2967 (4)  | 0.68761 (16)  | 0.0327 (7)                       |
| H4  | 0.2472        | 0.3728      | 0.6713        | 0.039*                           |
| C5  | 0.3856 (2)    | 0.2399 (4)  | 0.64723 (16)  | 0.0303 (7)                       |
| C6  | 0.4686 (3)    | 0.1275 (5)  | 0.67025 (17)  | 0.0377 (8)                       |
| H6  | 0.5244        | 0.0896      | 0.6423        | 0.045*                           |
| C7  | 0.4676 (3)    | 0.0724 (5)  | 0.73515 (18)  | 0.0425 (8)                       |
| H7  | 0.5237        | -0.0019     | 0.7514        | 0.051*                           |
| N1  | 0.3861 (3)    | 0.2978 (5)  | 0.57794 (16)  | 0.0402 (7)                       |
| H1F | 0.400 (3)     | 0.4157 (18) | 0.5742 (18)   | 0.041 (10)*                      |
| H1E | 0.438 (3)     | 0.248 (5)   | 0.5554 (19)   | 0.059 (13)*                      |
| H1D | 0.324 (2)     | 0.281 (6)   | 0.559 (2)     | 0.077 (16)*                      |
| O1  | 0.3897 (2)    | 0.0598 (4)  | 0.83889 (12)  | 0.0517 (7)                       |

*Atomic displacement parameters (Å<sup>2</sup>)*

|    | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$      |
|----|--------------|--------------|--------------|--------------|--------------|---------------|
| I1 | 0.04084 (17) | 0.04212 (17) | 0.04635 (17) | -0.00309 (9) | 0.01153 (9)  | -0.00348 (10) |
| C1 | 0.078 (3)    | 0.064 (3)    | 0.032 (2)    | 0.008 (2)    | 0.0061 (19)  | 0.0060 (18)   |
| C2 | 0.041 (2)    | 0.0286 (17)  | 0.0296 (17)  | -0.0015 (14) | -0.0032 (13) | 0.0018 (12)   |
| C3 | 0.0360 (17)  | 0.0326 (17)  | 0.0354 (18)  | 0.0031 (13)  | 0.0052 (14)  | -0.0018 (13)  |
| C4 | 0.0299 (16)  | 0.0293 (16)  | 0.0388 (18)  | 0.0051 (13)  | -0.0023 (13) | 0.0015 (13)   |
| C5 | 0.0321 (17)  | 0.0284 (16)  | 0.0303 (16)  | -0.0021 (12) | 0.0010 (12)  | 0.0009 (12)   |
| C6 | 0.0309 (17)  | 0.042 (2)    | 0.0404 (19)  | 0.0093 (14)  | 0.0065 (14)  | 0.0018 (15)   |

|    |             |             |             |             |              |             |
|----|-------------|-------------|-------------|-------------|--------------|-------------|
| C7 | 0.040 (2)   | 0.043 (2)   | 0.044 (2)   | 0.0164 (16) | -0.0033 (15) | 0.0045 (16) |
| N1 | 0.0400 (18) | 0.0456 (19) | 0.0352 (16) | 0.0018 (15) | 0.0045 (13)  | 0.0085 (14) |
| O1 | 0.0712 (19) | 0.0532 (16) | 0.0307 (13) | 0.0172 (13) | 0.0012 (12)  | 0.0097 (11) |

*Geometric parameters (Å, °)*

|             |            |             |            |
|-------------|------------|-------------|------------|
| C1—O1       | 1.407 (4)  | C4—H4       | 0.9300     |
| C1—H1A      | 0.9600     | C5—C6       | 1.380 (4)  |
| C1—H1B      | 0.9600     | C5—N1       | 1.466 (4)  |
| C1—H1C      | 0.9600     | C6—C7       | 1.375 (5)  |
| C2—O1       | 1.355 (4)  | C6—H6       | 0.9300     |
| C2—C3       | 1.383 (5)  | C7—H7       | 0.9300     |
| C2—C7       | 1.386 (5)  | N1—H1F      | 0.860 (10) |
| C3—C4       | 1.386 (5)  | N1—H1E      | 0.86 (4)   |
| C3—H3       | 0.9300     | N1—H1D      | 0.86 (3)   |
| C4—C5       | 1.371 (4)  |             |            |
| O1—C1—H1A   | 109.5      | C4—C5—N1    | 119.6 (3)  |
| O1—C1—H1B   | 109.5      | C6—C5—N1    | 119.0 (3)  |
| H1A—C1—H1B  | 109.5      | C7—C6—C5    | 119.0 (3)  |
| O1—C1—H1C   | 109.5      | C7—C6—H6    | 120.5      |
| H1A—C1—H1C  | 109.5      | C5—C6—H6    | 120.5      |
| H1B—C1—H1C  | 109.5      | C6—C7—C2    | 120.5 (3)  |
| O1—C2—C3    | 124.8 (3)  | C6—C7—H7    | 119.8      |
| O1—C2—C7    | 115.2 (3)  | C2—C7—H7    | 119.8      |
| C3—C2—C7    | 120.0 (3)  | C5—N1—H1F   | 111 (3)    |
| C2—C3—C4    | 119.5 (3)  | C5—N1—H1E   | 113 (3)    |
| C2—C3—H3    | 120.3      | H1F—N1—H1E  | 102 (3)    |
| C4—C3—H3    | 120.3      | C5—N1—H1D   | 113 (4)    |
| C5—C4—C3    | 119.7 (3)  | H1F—N1—H1D  | 105 (4)    |
| C5—C4—H4    | 120.1      | H1E—N1—H1D  | 111 (5)    |
| C3—C4—H4    | 120.1      | C2—O1—C1    | 118.8 (3)  |
| C4—C5—C6    | 121.3 (3)  |             |            |
| O1—C2—C3—C4 | -178.6 (3) | N1—C5—C6—C7 | -179.6 (3) |
| C7—C2—C3—C4 | 0.6 (5)    | C5—C6—C7—C2 | 0.9 (5)    |
| C2—C3—C4—C5 | 0.0 (5)    | O1—C2—C7—C6 | 178.2 (3)  |
| C3—C4—C5—C6 | -0.2 (5)   | C3—C2—C7—C6 | -1.1 (5)   |
| C3—C4—C5—N1 | 179.1 (3)  | C3—C2—O1—C1 | -10.9 (5)  |
| C4—C5—C6—C7 | -0.3 (5)   | C7—C2—O1—C1 | 169.8 (4)  |

*Hydrogen-bond geometry (Å, °)*

Cg1 is the centroid of the C2—C7 ring.

| <i>D</i> —H $\cdots$ <i>A</i>    | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N1—H1D $\cdots$ I1 <sup>i</sup>  | 0.86 (3)    | 2.67 (2)            | 3.503 (3)                  | 165 (5)                       |
| N1—H1F $\cdots$ I1 <sup>ii</sup> | 0.86 (1)    | 2.75 (2)            | 3.566 (3)                  | 159 (3)                       |
| N1—H1E $\cdots$ I1               | 0.86 (4)    | 2.75 (4)            | 3.568 (3)                  | 159 (4)                       |

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|                            |      |      |           |     |
|----------------------------|------|------|-----------|-----|
| C4—H4...Cg1 <sup>iii</sup> | 0.93 | 2.87 | 3.627 (4) | 140 |
| C7—H7...Cg1 <sup>iv</sup>  | 0.93 | 2.62 | 3.483 (4) | 155 |

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Symmetry codes: (i)  $x-1/2, -y+1/2, -z+1$ ; (ii)  $-x+1, -y+1, -z+1$ ; (iii)  $-x+1/2, y+1/2, z$ ; (iv)  $-x+1, y-1/2, -z+3/2$ .