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#### Key indicators

Single-crystal X-ray study  
 $T = 291$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.040  
 $wR$  factor = 0.062  
Data-to-parameter ratio = 19.1

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

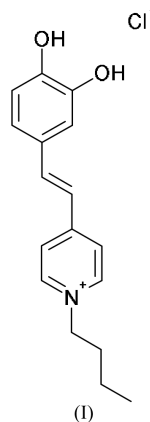
## *N*-Butyl-4-[2-(3,4-dihydroxyphenyl)vinyl]-pyridinium chloride

The crystal structure of the title compound,  $\text{C}_{17}\text{H}_{20}\text{NO}_2^+\cdot\text{Cl}^-$ , contains one molecule in the asymmetric unit. Molecules are linked *via* one  $\text{C}-\text{H}\cdots\text{O}$  and two  $\text{O}-\text{H}\cdots\text{Cl}$  hydrogen bonds. The molecule also contains one intramolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bond.

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#### Comment

As part of our investigations on organic photorefractive and electro-optical materials, we have determined the crystal structure of the title compound, (I) (Fig. 1).



The general synthetic procedure for this type of merocyanine dye was described by Okada *et al.* (1990) and further developed by Marder *et al.* (1990). It was suggested that this compound would be a good candidate for electro-optical and photorefractive applications.

#### Experimental

The title compound, (I), was prepared in a similar fashion to a general procedure reported by Dash & Mishra (1994). 3,4-Dihydroxybenzaldehyde (1.38 g, 10.0 mmol) and *N*-butyl-4-methylpyridinium chloride (1.85 g, 10.0 mmol) were dissolved in 30 ml anhydrous ethanol, with continuous stirring. To this solution, 2–3 drops of piperidine were added and the reaction mixture was refluxed and stirred for 5 h. After a few minutes, a dark-red solution was obtained. On completion of the reaction, the volume of the mixture was reduced under vacuum to a pasty mass, which was washed with acetone until a colourless acetone extract was obtained on washing. The residue was a dark-red solid mass which was then crystallized from rectified ethanol (yield 2.00 g, 62%). The purity of the new compound was confirmed by elemental analysis, IR, UV–vis and mass spectrometry. Crystals were grown from ethanol by slow evaporation at room temperature over a period of a week.

## Crystal data

 $C_{17}H_{20}NO_2^+ \cdot Cl^-$  $M_r = 305.79$ Monoclinic,  $P2_1/n$  $a = 7.6510$  (3) Å $b = 8.6180$  (3) Å $c = 24.5243$  (10) Å $\beta = 89.4079$  (15)° $V = 1616.96$  (11) Å<sup>3</sup> $Z = 4$  $D_x = 1.256$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation

Cell parameters from 12413

reflections

 $\theta = 2.8$ – $31.0^\circ$  $\mu = 0.24$  mm<sup>-1</sup> $T = 291$  (1) K

Plate, yellow

 $0.65 \times 0.15 \times 0.06$  mm

## Data collection

Nonius KappaCCD diffractometer

 $\omega$  scans at different  $\kappa$  angles

Absorption correction: none

11432 measured reflections

3684 independent reflections

1185 reflections with  $I > 2\sigma(I)$  $R_{int} = 0.080$  $\theta_{max} = 27.5^\circ$  $h = -9 \rightarrow 9$  $k = -9 \rightarrow 11$  $l = -31 \rightarrow 30$ 

## Refinement

Refinement on  $F^2$  $R[F^2 > 2\sigma(F^2)] = 0.040$  $wR(F^2) = 0.062$  $S = 0.81$ 

3684 reflections

193 parameters

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + 0.06P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{max} = 0.001$  $\Delta\rho_{max} = 0.32$  e Å<sup>-3</sup> $\Delta\rho_{min} = -0.22$  e Å<sup>-3</sup>

Table 1

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1–H1 <sup>i</sup> ···O2	0.82	2.23	2.6691 (19)	114
O1–H1 <sup>i</sup> ···Cl1	0.82	2.43	3.1742 (15)	151
O2–H2 <sup>i</sup> ···Cl1 <sup>i</sup>	0.82	2.20	3.0027 (13)	166
C11–H11 <sup>i</sup> ···O2 <sup>ii</sup>	0.93	2.38	3.297 (2)	170

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

H atoms were placed in calculated positions, with  $U_{iso}$  values were constrained to be 1.5 times  $U_{eq}$  of the carrier atom for the methyl and hydroxy H atoms, and 1.2 times  $U_{eq}$  for the other H atoms. The methyl and hydroxy groups were allowed to rotate but not to tip.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*, *PARST95* (Nardelli, 1995) and *PLATON* (Spek, 2001).

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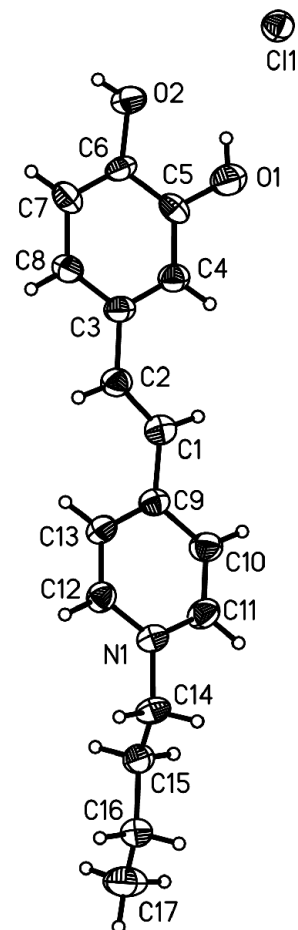


Figure 1

View of the title compound, showing the labelling of all non-H atoms. Displacement ellipsoids are shown at the 30% probability level.

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