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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.006 Å
R factor = 0.041
wR factor = 0.102
Data-to-parameter ratio = 18.6

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

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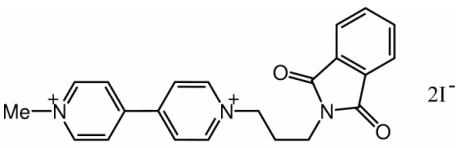
The asymmetric unit of the title compound, $C_{22}H_{21}N_3O_2^{2+}\cdot 2I^-$, consists of a substituted bipyridinium cation and two iodide anions. The dihedral angle between the two rings within the phthalimide moiety is 1.7 (3)°, where the r.m.s. deviations for the five- and six-membered rings are 0.006 and 0.004 Å, respectively. On the other hand, the two pyridinium rings are tilted at an angle of 3.9 (3)° because of the steric contacts between the H atoms at the 3-, 5-, 3′- and 5′-positions of the 4,4′-bipyridinium moiety. The phthalimide plane is tilted by 68.5 (1)° with respect to the pyridinium plane, directly attached to the propylene moiety.

Comment

A photochemical system made up of $Ru(bpy)_3^{2+}$ (bpy = 2,2′-bipyridine) and methylviologen (usually, *N*,*N*′-dimethyl-4,4′-bipyridinium dichloride) has been thought of as one of the promising candidates to achieve artificial photosynthetic devices. We previously reported that some amidate-bridged platinum dimers with the general formula $[Pt_2(NH_3)_4(\mu\text{-amidato})_2]^{2+}$ (amidate = acetamidate, α-pyrrolidinonate, α-pyridonate, *etc*.) serve as effective H_2-producing catalysts in a well known photosystem consisting of edta, $Ru(bpy)_3^{2+}$ and methylviologen (Sakai *et al.*, 1993). Since then, various efforts have been made to develop a more effective system in which the chemical species mentioned above are linked together to give a single molecular device. The title compound, (I), was obtained as a precursor in such studies.



(I)

The molecular structure and the crystal packing diagram for (I) are shown in Figs. 1 and 2, respectively. All bond distances and angles in (I) are in the expected ranges.

Experimental

A solution of *N*-methyl-4,4′-bipyridinium iodide (1.0 mmol; Van Emon *et al.*, 1986) and *N*-(3-bromopropyl)phthalimide (1.1 mmol) in methanol (20 ml) was refluxed for 2 d. The red prisms or plates deposited were collected by filtration and air-dried (yield: 52%). The purity has been checked by ^{1}H NMR spectroscopy.

Crystal data

$C_{22}H_{21}N_3O_2^{2+}\cdot 2I^-$	$Z = 2$
$M_r = 613.22$	$D_x = 1.775$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 6.0535$ (5) Å	Cell parameters from 3414 reflections
$b = 7.4674$ (6) Å	$\theta = 2.8$–$27.2°$
$c = 25.776$ (2) Å	$\mu = 2.76$ mm^{-1}
$\alpha = 83.715$ (1)°	$T = 296$ (2) K
$\beta = 88.570$ (2)°	Plate, red
$\gamma = 82.223$ (1)°	0.20 × 0.20 × 0.05 mm
$V = 1147.45$ (16) Å^3	

Data collection

Bruker SMART APEX CCD-detector diffractometer	4883 independent reflections
ω scans	4060 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.019$
$T_{min} = 0.586$, $T_{max} = 0.871$	$\theta_{max} = 27.5°$
6983 measured reflections	$h = -7 \rightarrow 7$
	$k = -8 \rightarrow 9$
	$l = -24 \rightarrow 33$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.5905P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.041$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.102$	$\Delta\rho_{max} = 1.27$ e Å^{-3}
$S = 1.05$	$\Delta\rho_{min} = -0.44$ e Å^{-3}
4883 reflections	
263 parameters	
H-atom parameters constrained	

All H atoms were located at their idealized positions as riding atoms [C—H(aromatic) = 0.93 Å, C—H(methylene) = 0.97 Å and C—H(methyl) = 0.96 Å]. In the final difference Fourier synthesis, five residual peaks in the range 1.01–1.27 e Å^{-3} were observed within 0.94 Å of I atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *KENX* (Sakai, 2002); software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997), *TEXSAN* (Molecular Structure Corporation, 2001), KENX (Sakai, 2002) and *ORTEP*II (Johnson, 1976).

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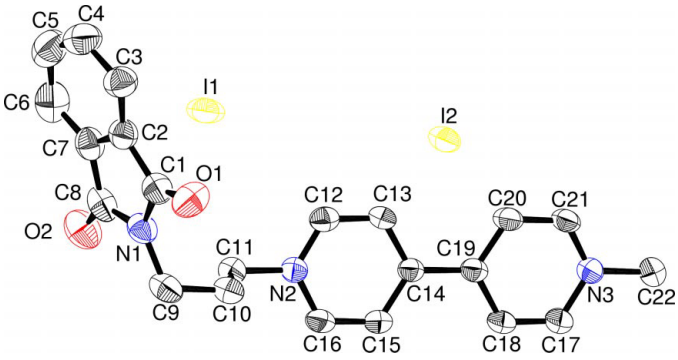

Figure 1
The structure of the independent cation and anions in (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

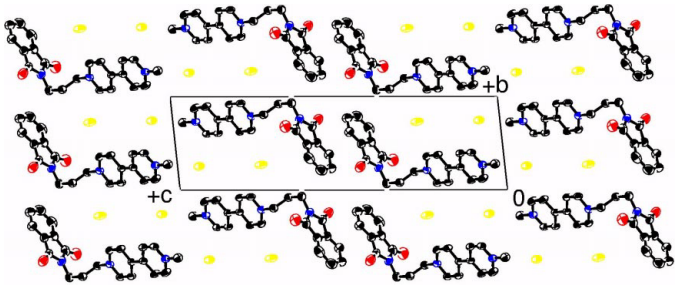

Figure 2
Crystal packing, viewed down the *a* axis of (I).

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