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2-(4-Pyridinio)benzimidazolium tetrachloridopalladium(II)

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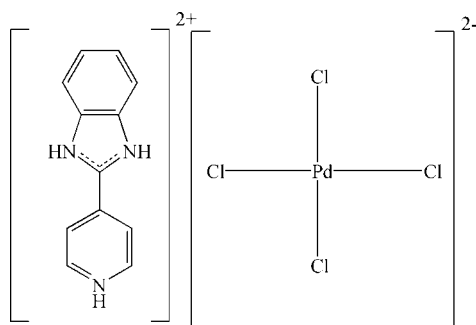
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.030; wR factor = 0.074; data-to-parameter ratio = 18.5.

The asymmetric unit of the title compound, $(\text{C}_{12}\text{H}_{11}\text{N}_3)^+$ - $[\text{PdCl}_4]^-$, consists of a 2-(4-pyridinio)benzimidazolium cation and two half $[\text{PdCl}_4]^{2-}$ anions, which are located on inversion centres. The cations lie in sheets parallel to $(\bar{2}1\bar{2})$. The cations and anions are connected by $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{C}-\text{H}\cdots\text{Cl}$ contacts.

Related literature

For related structures, see: Alcade *et al.* (1992); Chen *et al.* (2006); Huang *et al.* (2004); Wang *et al.* (1999).



Experimental

Crystal data

$(\text{C}_{12}\text{H}_{11}\text{N}_3)[\text{PdCl}_4]$
 $M_r = 445.44$
 Triclinic, $P\bar{1}$

$a = 8.2221$ (1) Å
 $b = 8.3964$ (2) Å
 $c = 12.3768$ (5) Å

$\alpha = 94.09$ (3)°
 $\beta = 97.42$ (2)°
 $\gamma = 116.102$ (10)°
 $V = 752.95$ (11) Å³
 $Z = 2$

Mo $K\alpha$ radiation
 $\mu = 1.93$ mm⁻¹
 $T = 293$ (2) K
 $0.30 \times 0.15 \times 0.04$ mm

Data collection

Rigaku Mercury CCD diffractometer
 Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)
 $T_{\min} = 0.713$, $T_{\max} = 0.916$

5851 measured reflections
 3406 independent reflections
 2816 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.074$
 $S = 1.06$
 3406 reflections

184 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.81$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.61$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{Cl4}$	0.86	2.55	3.207 (3)	134
$\text{N2}-\text{H2A}\cdots\text{Cl3}^{\text{i}}$	0.86	2.32	3.165 (2)	167
$\text{N3}-\text{H3A}\cdots\text{Cl1}$	0.86	2.28	3.138 (3)	172
$\text{C5}-\text{H5A}\cdots\text{Cl1}^{\text{ii}}$	0.93	2.64	3.556 (3)	167

Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 1, -y + 1, -z$.

Data collection: *CrystalClear* (Rigaku, 2002); 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: *DIAMOND* (Brandenburg & Putz, 2006) and *SHELXTL* (Sheldrick, 2008); 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: BT2834).

References

- Alcade, E., Dinares, I., Perez-Garia, L. & Roca, T. (1992). *Synthesis*, pp. 295–398.
 Brandenburg, K. & Putz, H. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
 Chen, L. J., He, X., Xia, C. K., Zhang, Q. Z., Chen, J. T., Yang, W. B. & Lu, C. Z. (2006). *Cryst. Growth Des.* **9**, 2076–2085.
 Huang, X.-C., Zeng, M.-H. & Ng, S. W. (2004). *Acta Cryst.* **E60**, o939–o940.
 Rigaku (2002). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Wang, Z. Y., Wilson, S. R., Foxman, B. M. & Lin, W. B. (1999). *Cryst. Eng.* **2**, 91–100.

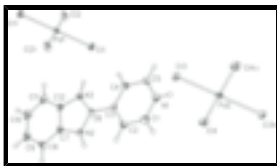
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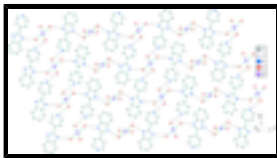
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