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(*p*-Phenylenedimethylene)diammonium dichloride

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Key indicators

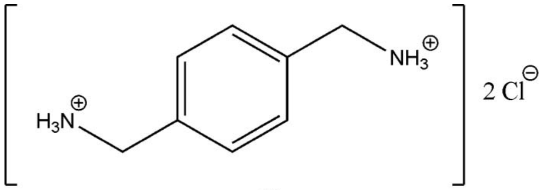
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.092
Data-to-parameter ratio = 11.9

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

In the title compound, $C_8H_{14}N_2^{2+}\cdot 2Cl^-$, the cation possesses a crystallographically imposed center of symmetry. The crystal packing is stabilized by intermolecular N—H···Cl hydrogen bonds and π–π stacking interactions.

Comment

There is an interest in novel semiconductors that are more versatile than the current Si-based devices. Research has been carried out on organic semiconductors such as pentacene (Jurchescu *et al.*, 2004; de Boer *et al.*, 2004), which have the advantage that they are flexible and possibly inkjet printable. However, due to the weak van der Waals bonding, these materials have a limited carrier mobility. The properties of the organics can be improved by combining them with inorganics in hybrid materials (Mitzi, 1999). We present here the crystal structure of the title compound, (I), which we use as the starting point for the development of new hybrids.



(I)

In (I) (Fig. 1), all bond lengths and angles show normal values (Allen *et al.*, 1987). The cations lie on centers of symmetry and form stacks parallel to the *a* axis, with a short

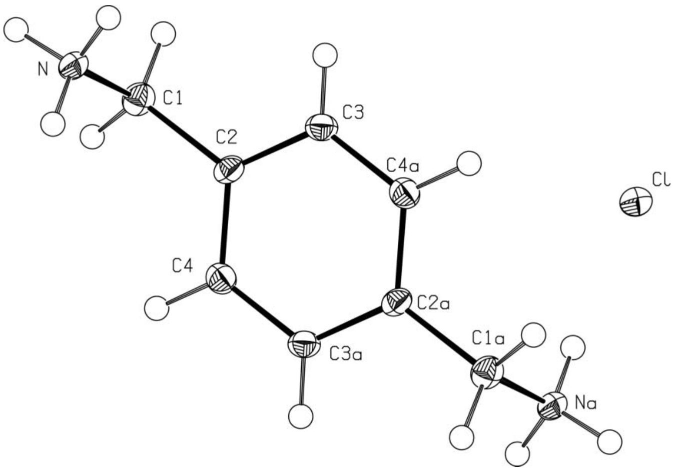


Figure 1
The molecular structure of (I), showing the atomic labeling and 50% probability displacement ellipsoids [symmetry code: (*a*) $1 - x, -y, 1 - z$].

C2$\cdots$C4^{iv} distance of 3.496 (2) Å [symmetry code: (iv) $x + 1, y, z$], suggesting π–π stacking interactions. Intermolecular N—H$\cdots$Cl hydrogen bonds (Table 1) contribute to the stability of the crystal packing (Fig. 2).

Experimental

α,α'-Diamino-*p*-xylene (2 g, Fluka, purum > 98%) was dissolved in water (7 ml). Subsequently, saturated (37%) HCl (5 ml, Merck) was added with stirring and cooling on a water bath. The mixture was filtered and the resulting white powder was washed with water and dried in air. Small colorless crystals were obtained by recrystallization from a saturated aqueous solution at 343 K, which was slowly cooled to room temperature.

Crystal data

$C_8H_{14}N_2^{2+}\cdot 2Cl^-$
$M_r = 209.12$
Triclinic, $P\overline{1}$
$a = 4.3496$ (8) Å
$b = 5.809$ (1) Å
$c = 10.197$ (2) Å
$\alpha = 101.836$ (3)°
$\beta = 99.727$ (3)°
$\gamma = 93.800$ (3)°
$V = 247.18$ (8) Å^3
$Z = 1$
$D_x = 1.405$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.61$ mm^{-1}
$T = 100$ (1) K
Platelet, colorless
0.17 × 0.08 × 0.03 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2006)
$T_{min} = 0.900$, $T_{max} = 0.982$
1835 measured reflections
986 independent reflections
881 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 26.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.092$
$S = 1.06$
986 reflections
83 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0368P)^2 + 0.28P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N—H5$\cdots$Cl^{i}	0.92 (3)	2.32 (3)	3.190 (2)	158 (3)
N—H5′$\cdots$Cl^{ii}	0.92 (3)	2.32 (3)	3.235 (2)	176 (2)
N—H5″$\cdots$Cl^{iii}	0.93 (4)	2.28 (4)	3.199 (2)	175 (4)

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

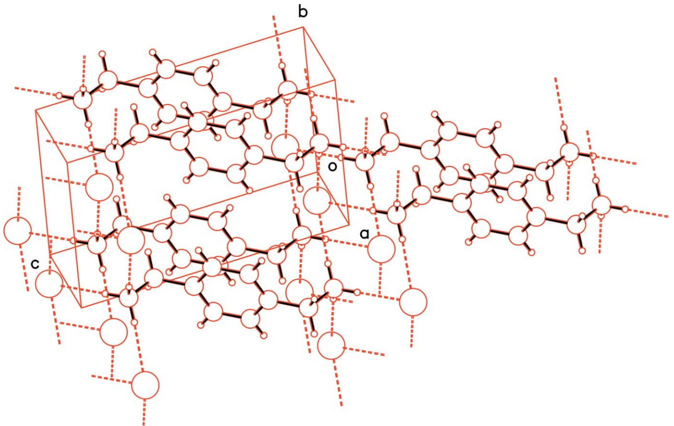


Figure 2
A portion of the crystal packing, showing the N—H$\cdots$Cl hydrogen bonds as dashed lines.

All H atoms were located in a difference Fourier map and refined with isotropic displacement parameters [O—H = 0.92 (3)–0.98 (3) Å].

Data collection: *SMART* (Bruker, 2006); cell refinement: *SAINT-Plus* (Bruker, 2006); data reduction: *SAINT-Plus*; program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLUTO* (Meetsma, 2006) and *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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