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2,2′-(*p*-Phenylenediimino)dipyridinium dichloride hexahydrate

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In the crystal structure of the title compound, $C_{16}H_{16}N_4^{2+}\cdot 2Cl^-\cdot 6H_2O$, the 2,2′-(*p*-phenylenediimino)-dipyridinium cation has inversion symmetry. The chloride ions and water molecules are linked *via* O—H···O and O—H···Cl$^-$ hydrogen bonds into an infinite two-dimensional network parallel to the (001) plane. The cations, as fourfold hydrogen-bond donors, connect neighbouring $[Cl^-\cdot(H_2O)_3]_\infty$ anionic networks into polymeric three-dimensional hydrogen-bonded assemblies.

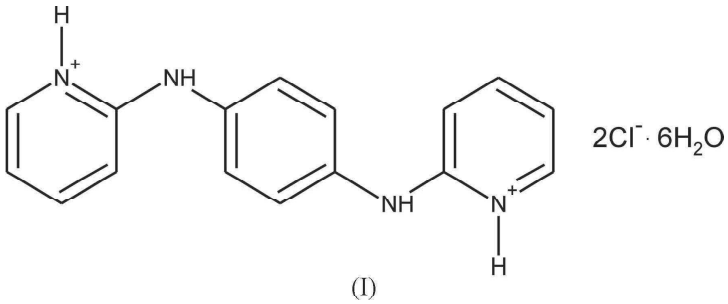
Key indicators

Single-crystal X-ray study
T = 170 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.101
Data-to-parameter ratio = 13.7

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

Comment

N,*N*′-Bis(2-pyridyl)aryldiamines with two proton-donor and two proton-acceptor sites have been used as versatile substrates in the synthesis of extended supramolecular arrays (Bensemann *et al.*, 2002, 2003; Gdaniec *et al.*, 2002, 2005). Whereas *N*,*N*′-bis(2-pyridyl)aryldiamines cocrystallize relatively easily with dicarboxylic acids, forming good-quality crystals consisting of predictable one-dimensional hydrogen-bond assemblies (Bensemann *et al.*, 2003), their salts with simple inorganic acids, with only a few exceptions, are difficult to crystallize. Here, we report the crystal structure of 2,2′-(*p*-phenylenediimino)dipyridinium dichloride hexahydrate, (I), which was obtained as an intermediate product in the synthesis of *N*,*N*′-di-2-pyridylbenzene-1,4-diamine (PDAB).



(I)

The asymmetric unit of (I) consists of one half of the centrosymmetric PDAB dication, one chloride ion and three water molecules (Fig. 1). In the crystalline state, PDAB has been observed in a variety of conformations, ranging from a nearly planar *Z*,*Z* form in its cocrystal with phenazine (Gdaniec *et al.*, 2005) to strongly twisted *Z*,*Z* and *E*,*E* forms in its polymorphs (Bensemann *et al.*, 2002). It was obvious that, for steric reasons, double protonation of the PDAB occurring at the pyridine N atoms should force the dication to adopt a non-planar conformation. In (I), the pirydynium and benzene units are inclined at an angle of 51.85 (9)°. They are rotated with respect to the C2/N2/C7 plane; however, as in the free base, the twist about the N2—C_{ar} bond is significantly smaller

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