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2,6-Diamino-4-phenyltriazinium chloride monohydrate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.077
Data-to-parameter ratio = 16.6

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

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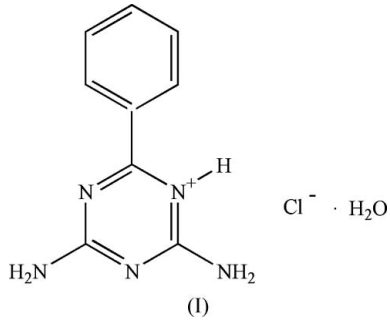
The asymmetric unit of the title compound, $C_9H_{12}ClN_5O$, contains one cation, one anion, and one water molecule. Intermolecular N—H···N, N—H···O, N—H···Cl and O—H···Cl hydrogen bonds seem to be effective in the stabilization of the crystal structure, resulting in the formation of a three-dimensional framework.

Comment

Hydrogen bonds are often applied to model systems in the study of proton-transfer reactions. An advantage of using such specific systems is the enhanced structural and thermodynamic stabilities of hydrogen bonds. Intramolecular hydrogen bonds stabilize the folded form of proteins as well as small organic molecules. Although proton transfer in the gas phase or in solution has been studied extensively, it has been scarcely explored in the solid state. We have previously reported some self-associated proton-transfer systems, using pyridine-2,6-dicarboxylic acid ($pydcH_2$), 1,10-phenanthroline-2,9-dicarboxylic acid ($phendcH_2$) and 4-hydroxy-pyridine-2,6-dicarboxylic acid ($hypydcH_2$) as proton donors, and 2,6-pyridinediamine (pyda), creatinine (creat), *N*,*N*′-diethyl-2-amino-6-metyl-4-pyrimidinol (pyrim), guanidine (G), 1,10-phenanthroline (phen) and guanidine hydrochloride (GHCl) as proton acceptors; these formed the proton-transfer compounds (creatH)(pydcH) (Moghimi, Sharif *et al.*, 2004), (creatH)(phendcH) (Soleimannejad *et al.*, 2005), (pydaH)(pydcH) (Aghabozorg, Akbari Saei *et al.*, 2005), (pyrimH){H(Hpydc)$_2$} (Aghabozorg, Soleimannejad *et al.*, 2005), (GH)(hypydcH)·H_2O (Moghimi, Aghabozorg *et al.*, 2005), $(phenH)_2(pydc)$ (Moghimi, Sheshmani *et al.*, 2005) and $(GH)_2(pydc)$ (Moghimi, Sheshmani *et al.*, 2004). We report here the synthesis and crystal structure of the title self-associated system, arising from ion-pairing and hydrogen bonding.



(I)

In the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The forces between cations and anions consist of hydrogen bonding and

ion-pairing. The intermolecular N—H···N, N—H···O, N—H···Cl and O—H···Cl hydrogen bonds (Table 1) seem to be effective in the stabilization of the crystal structure, resulting in the formation of a three-dimensional framework (Fig. 2).

Experimental

An aqueous solution of 2,6-diamino-4-phenyltriazine (935 mg, 5 mmol) in dimethyl sulfoxide (50 ml) was added to a solution of hydrochloric acid (0.42 ml, 5 mmol). Light-orange prismatic crystals of (I) were obtained by slow evaporation of the solvent at room temperature after ten weeks (yield 70%, m.p. 573 K).

Crystal data

$C_9H_{10}N_5^+\cdot Cl^-\cdot H_2O$
M_r = 241.69
Monoclinic, $P2_1/c$
a = 8.4122 (9) Å
b = 5.0193 (5) Å
c = 26.333 (3) Å
β = 93.486 (2)°
V = 1109.8 (2) Å^3
Z = 4
D_x = 1.446 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 294 (2) K
Prism, light orange
0.2 × 0.16 × 0.14 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.937, T_{max} = 0.957
8092 measured reflections
2414 independent reflections
1847 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.077
S = 1.02
2414 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.01P)^2 + 0.65P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H1···N1^{i}	0.87	2.18	3.031 (2)	166
N7—H2···O1^{ii}	0.87	2.32	2.955 (2)	130
N5—H3···Cl1^{iii}	0.87	2.37	3.166 (2)	153
N8—H4···O1^{iv}	0.87	2.08	2.945 (2)	178
N8—H5···Cl1^{iii}	0.87	2.45	3.264 (2)	156
O1—H6···Cl1^{v}	0.87	2.31	3.136 (2)	159
O1—H7···Cl1^{vi}	0.94	2.42	3.252 (2)	148

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $-x+2, -y+2, -z+1$; (iii) $x, y-1, z$; (iv) $x, y-1, z-1$; (v) $-x+1, -y+2, -z+1$; (vi) $-x+1, -y+1, -z+1$.

H atoms of the water, NH_2 and NH groups were located in difference syntheses and refined as riding with distances of O—H = 0.87–0.94 Å, N—H = 0.87 Å and U_{iso}(H) = 1.2U_{eq}(N,O). The remaining H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

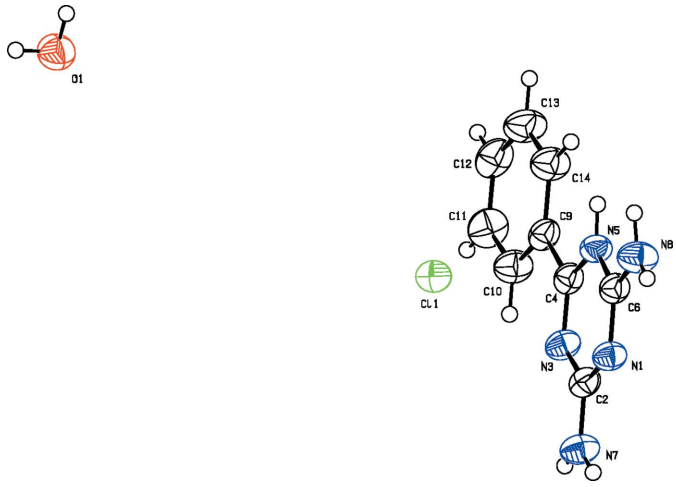


Figure 1
The asymmetric unit of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

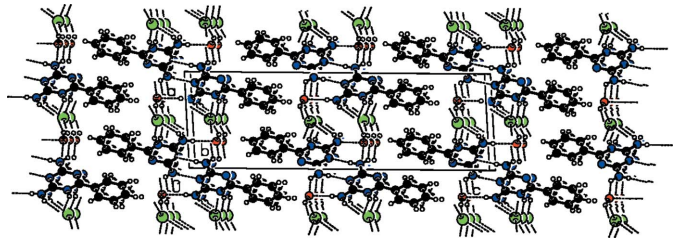


Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

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References

Aghabozorg, H., Akbari Saei, A. & Ramezanipour, F. (2005). *Acta Cryst.* E**61**, o3242–o3244.
Aghabozorg, H., Soleimannejad, J., Sharif, M. A., Sheshmani, S. & Moghimi, A. (2005). *Anal. Sci.* **21**, x73–x74.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–19.
Bruker (1998). *SAINT-Plus* (Version 6.01) and *SMART* (Version 5.059). Bruker AXS Inc., Madison, Wisconsin, USA.
Moghimi, A., Aghabozorg, H., Sheshmani, S. & Soleimannejad, J. (2005). *Anal. Sci.* **21**, x71–x72.
Moghimi, A., Sharif, M. A. & Aghabozorg, H. (2004). *Acta Cryst.* E**60**, o1790–o1792.
Moghimi, A., Sheshmani, S., Shokrollahi, A., Aghabozorg, H., Shamsipur, M., Kickelbick, G., Carla Aragoni, M. & Lippolis, V. (2004). *Z. Anorg. Allg. Chem.* **630**, 617–624.
Moghimi, A., Sheshmani, S., Shokrollahi, A., Shamsipur, M., Kickelbick, G. & Aghabozorg, H. (2005). *Z. Anorg. Allg. Chem.* **631**, 160–169.
Sheldrick, G. M. (1998). *SADABS* (Version 2.01) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Soleimannejad, J., Sharif, M., Sheshmani, S., Alizadeh, R., Moghimi, A. & Aghabozorg, H. (2005). *Anal. Sci.* **21**, x49–x50.